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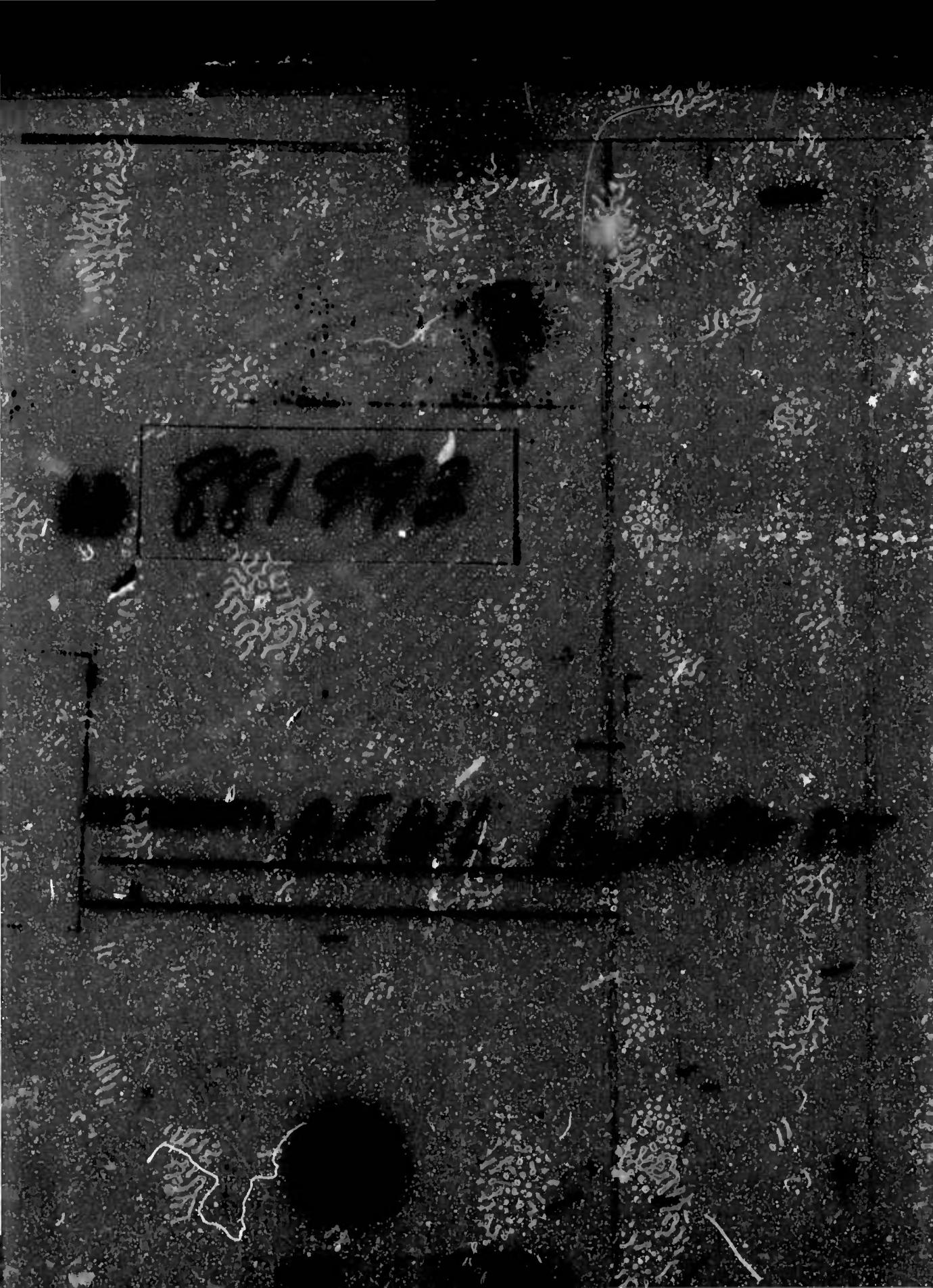
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FRANCK-CONDON FACTORS FOR VARIOUS AIR SPECIES

John I. Generosa
Major USAF

Richard A. Harris
Captain USAF

Louis R. Sullo
Lt USAF

TECHNICAL REPORT NO. AFWL-TR-70-108

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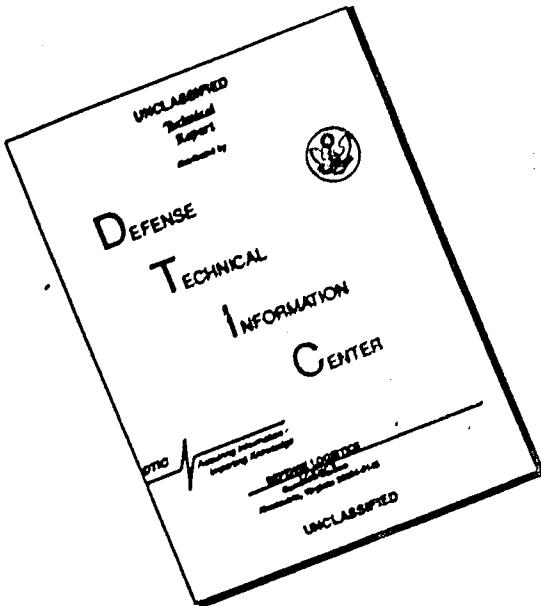
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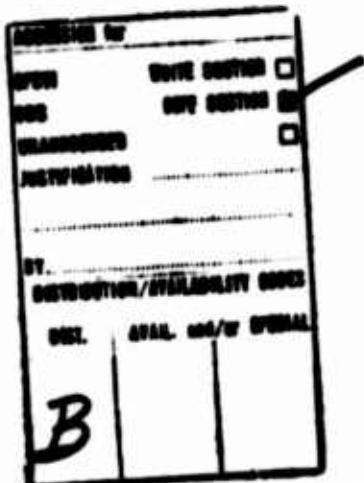
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FOREWORD

This research was performed under Program Element 61102H, Project 5710, Subtask HC 061, and was funded by the Defense Atomic Support Agency (DASA).

Inclusive dates of research were July 1967 through September 1968. The report was submitted 27 November 1970 by the Air Force Weapons Laboratory Project Officer, Captain Richard Harris (SYT).

This technical report has been reviewed and is approved.

Richard A. Harris

RICHARD A. HARRIS
Captain, USAF
Project Officer

Brown B. Rogers

BROWN B. ROGERS
Major, USAF
Chief, Theoretical Physics Branch

Carl B. Hilland

CARL B. HILLAND
Lt Colonel, USAF
Chief, Technology Division

ABSTRACT

(Distribution Limitation Statement No. 3)

In the process of calculating opacities which are needed as input data for radiation transport problems, the absorption cross sections for various species has to be known. One factor in the cross section is the vibrational transition probability, called the Franck-Condon factor (FCF). This report presents input data needed to calculate these from Rydberg-Klein potentials as well as tables of Franck-Condon factors for species of atmospheric interest.

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LIST OF VARIABLES

B_e	rotational constant in the equilibrium position
B_i	rotational constant used by Vanderslice for the i^{th} level determined by least squares fit
B_v	rotational constant for the v^{th} vibrational level
B_v^{eff}	effective rotational constant for the v vibrational level
D_e	dissociation energy of the electronic state of the molecule
dt	volume element
$E(I,K)$	vibrational-rotational energy of a molecule in terms of continuous classical variables, I,K
$E(v,J)$	vibrational-rotational energy of a molecule in terms of vibrational and rotational quantum numbers
E_R	rotational energy of a molecule
E_v	vibrational energy of a molecule
f	a Klein action integral: $\partial S / \partial U$
g	a Klein action integral: $-\partial S / \partial K$
G_v	vibrational term
$\Delta G_{v+\frac{1}{2}}$	separation of successive vibrational terms
\hat{H}	Hamiltonian operator
I	classical action integral, when quantized it is set equal to $\hbar(v+\frac{1}{2})$
I'	the value of I such that $U = E(I,K)$
J	rotational quantum number
K	related to classical angular momentum
l	classical angular momentum
m	mass
O_p	a general operator of quantum mechanics
p_r	linear momentum along r (internuclear separation) axis
$q_{v'v''}$	Franck-Condon factor
r	internuclear separation of molecule

LIST OF VARIABLES (cont'd)

r_e	internuclear separation at equilibrium
r_{\max}	larger of the two classical turning points
r_{\min}	smaller of the two classical turning points
$r_{v'v''}$	r centroid
$r^2_{v'v''}$	r^2 centroid
$S(U,K)$	Klein's auxiliary function
τ	total transition probability
T_e	relative energy of separation between the minimums of two electronic states
U	total vibrational-rotational energy of a molecule
U_i	energy of the i^{th} level in Vanderslice's formulation
v	vibrational quantum number
$V(r)$	rotationless vibrational potential of a molecule
V_{eff}	rotationless vibrational potential corrected for centrifugal effects
w_i	parameter in Vanderslice's formulation
α_e	rotational constant
γ_e	rotational constant
δ_e	rotational constant
ϵ_e	rotational constant
μ	reduced mass of molecule
ψ_f	final total wave function
ψ_i	initial total wave function
ψ_{fe}	final electronic wave function
ψ_{ie}	initial electronic wave function
ψ_{fR}	final rotational wave function
ψ_{iR}	initial rotational wave function
ψ_{fv}	final vibrational wave function

LIST OF VARIABLES (cont'd)

ψ_{iv}	initial vibrational wave function
$\psi_{v''}$	vibrational wave function for lower state
$\psi_{v'}$	vibrational wave function for upper state
t_v	period of vibration of molecule
w_e	vibrational constant
w_{exe}	vibrational constant
w_{eye}	vibational constant
w_{eze}	vibrational constant
w_{ete}	vibrational constant
w_i	vibrational constant in Vanderslice's formulation determined from least squares fit
w_{ixi}	vibrational constant in Vanderslice's formulation determined from least squares fit

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SECTION I
INTRODUCTION

For any given fixed temperature, the intensity distribution of the spectrum of a band system in a typical atmospheric diatomic molecule is determined primarily by the vibrational transition probability. The intensity distribution within a vibrational band is determined by the rotational transition probability. This report will be concerned with only the calculation of the vibrational transition probabilities called the Franck-Condon factors. These are defined by the following overlap integral:

$$q_{v'v''} = \left(\int \psi_{v'} \psi_{v''} dr \right)^2 \quad (1)$$

where $\psi_{v'}$, $\psi_{v''}$ are the vibrational wave functions to be described in detail later and v' , v'' refer to the upper and lower vibrational quantum number, respectively. The Franck-Condon factors satisfy the following relations:

$$\text{all } \sum_{v'} q_{v'v''} = 1$$

and

$$\text{all } \sum_{v''} q_{v'v''} = 1 \quad (2)$$

Since the overlap integral involves the vibrational wavefunctions of the initial and final states of the molecule, the Schrodinger equation must be solved for these wavefunctions.

$$\hat{H} \psi_v = E_v \psi_v \quad (3)$$

where

ψ_v is the vibrational wavefunction of level v

E_v is the energy of vibrational level v

\hat{H} is the Hamiltonian operator for the problem

The Hamiltonian operator contains a term for the potential energy in which the two nuclei move. The correctness of this potential will determine how good the vibrational wavefunctions will be. This in turn determines the accuracy of the Franck-Condon factors. Hence the better the potential the better the Franck-Condon factors.

There have been a great many empirical potential energy functions developed over the past few decades. A study of these and the relative merits of each has been done by Steele et al. (Ref. 1).

Among the most popular potentials in the past for calculating Franck-Condon factors has been the Morse potential.

$$V(r) = De \left[1 - e^{-ax} \right]^2 \quad (4)$$

where

$$a = \sqrt{\frac{4\pi^2 c^2 \omega e^2 u}{2De}}$$

De is the dissociation energy

$$x = (r - r_e)$$

r_e is the internuclear separation at the minimum of the potential well

r is the internuclear separation

Using this potential one can develop a closed form representation for the wavefunctions, hence the evaluation of the overlap integrals can be done without the need of a large computer. However, this potential is accurate only near the bottom of the potential well. Therefore the Franck-Condon factors for the upper vibration levels may be inaccurate.

To calculate better wavefunctions for the upper vibrational levels, one needs a better potential. One such method for calculation a better potential has been developed by Rydberg (Ref. 2) and Klein (Ref. 3), which makes use of experimentally measured data. Subsequently, it has been modified in various ways by other investigators, notably by Rees (Ref. 4). The general method has become known as the Rydberg-Klein-Rees or R-K-R method. In many instances this is a misnomer because the Rees modification is not even used.

The method is based on a WKB approximation and will be outlined below. This treatment of the basic equations is based on the derivation in a paper by Vanderslice et al. (Ref. 5).

Rydberg used two expressions from classical mechanics and modified them appropriately to obtain the corresponding quantum mechanical expressions. The classical equations for the action integral is

$$\int p_r dr = (2\mu)^{1/2} \int [\tilde{U} - \tilde{V}_{eff}]^{1/2} dr \quad (5)$$

where

p_r is the momentum in r direction

r is the internuclear separation

μ is the reduced mass of the molecule

\tilde{V}_{eff} is the effective potential

\tilde{U} is the total vibrational-rotational energy given by

$$\tilde{U} = \frac{(p_r)^2}{2\mu} + \frac{\ell^2}{2\mu r^2} + \tilde{V}(r) \quad (6)$$

where

ℓ is the angular momentum of the rotating molecule

$\tilde{V}(r)$ is the potential energy of the rotationless molecule

Letting

$$K = \frac{\ell^2}{2\mu}$$

one then has

$$\tilde{U} = \frac{(p_r)^2}{2\mu} + \frac{K}{r^2} + \tilde{V}(r)$$

or

$$\tilde{U} = \frac{p_r^2}{2\mu} + \tilde{V}_{eff} \quad (7)$$

where

$$\tilde{V}_{\text{eff}} = \frac{K}{r^2} + \tilde{V}(r)$$

from which follows equation (7) after solving the P_r and substituting this expression in the action integral.

The action integral equation (17) is quantized as if it were a harmonic oscillator which results in the equation

$$\hbar(v+\frac{1}{2}) = (2\mu)^{\frac{1}{2}} \int [\tilde{U} - \tilde{V}_{\text{eff}}]^{\frac{1}{2}} dr \quad (8)$$

This is the first basic equation of Rydberg's method.

The second basic equation of Rydberg involves the rotational energy of the system. Again, classically this is given by

$$\tilde{E}_r = K \left(\frac{1}{r^2} \right)_v = \frac{K}{\tau_v} \int \left(\frac{1}{r^2} \right) dt = \frac{K}{\tau_v} \int \frac{1}{r^2 P_r} dr \quad (9)$$

where

K is the same as for equation (7)

τ_v is the period of vibration

Quantization of K the rotational angular momentum leads to

$$K = \frac{\hbar^2}{8\pi^2\mu} J(J+1) \quad (10)$$

with which the rotational energy integral becomes, upon solving equation (15) for P_r and substituting this in equation (17),

$$\frac{\hbar^2}{8\pi^2\tau} \frac{1}{\sqrt{2\mu}} \int [\tilde{U} - \tilde{V}_{\text{eff}}]^{-\frac{1}{2}} \frac{dr}{r^2} = \frac{\hbar^2}{8\pi^2\mu} \left(\frac{1}{r^2} \right)_v = B_v \quad (11)$$

This is Rydberg's second basic equation. Rydberg solved these graphically. The second of these becomes infinite at the classical turning points since $\tilde{U} = \tilde{V}_{\text{eff}}$ there. This increases the difficulty of solving the problem graphically since large errors can be made in the regions of the classical turning points.

Klein defined a new function $S(\tilde{U}, K)$ to aid in finding the classical turning points, given by

$$S(\tilde{U}, K) = \frac{1}{(2\pi^2 v)^{\frac{1}{2}}} \int_0^{I'} [\tilde{U} - \tilde{E}(I, K)]^{\frac{1}{2}} dI \quad (12)$$

where

$$I = h(v + \frac{1}{2})$$

\tilde{U} is the total energy

$$K = \frac{\ell^2}{2\mu}$$

$\tilde{E}(I, K)$ is the vibrational-rotational energy

I' is the value of I such that $\tilde{U} = \tilde{E}(I, K)$

Using this function Klein found that expressions for the classical turning points were given by

$$\frac{\partial S}{\partial \tilde{U}} = f = \frac{1}{2} (r_{\max} - r_{\min}) \quad (13)$$

and

$$-\frac{\partial S}{\partial K} = g = \frac{1}{2} \left(\frac{1}{r_{\min}} - \frac{1}{r_{\max}} \right) \quad (14)$$

which can be inverted to give

$$r_{\min} = \left(\frac{f}{g} + f^2 \right) - f \quad (15)$$

$$r_{\max} = \left(\frac{f}{g} + f^2 \right) + f \quad (16)$$

The integration and differentiation of Klein's equations must be carried out numerically in general. Before the large computers of recent years this presented a problem. Rees therefore made the next modification to the Rydberg-Klein method, by observing that the integral for $S(\tilde{U}, K)$ could be integrated analytically if in the function $\tilde{E}(I, K)$, I is expressable as a quadratic (or cubic) form in $(v + \frac{1}{2})$. Consequently, f, g can be written in closed form.

Vanderslice et al. capitalized on this observation and have fitted the energy $\tilde{E}(I, K)$ with a series of quadratics over the whole energy range of the potential function. They then obtained a closed form representation for g, f

and consequently, r_{\min} and r_{\max} . Their expressions for g and f are

$$f = \left(\frac{h}{8\pi^2 \mu c} \right)^{\frac{1}{2}} \sum_{i=1}^n (wx)_i^{-\frac{1}{2}} \ln w_i \quad (17)$$

$$g = \left(\frac{2\pi^2 \mu c}{h} \right)^{\frac{1}{2}} \sum_{i=1}^n \left[\frac{1}{4} \alpha_i (wx)_i^{-1} \left(U_i^{\frac{1}{2}} - U_{i-1}^{\frac{1}{2}} \right) + (wx)_i^{-\frac{1}{2}} \left(2B_i - \alpha_i (wx)_i^{-1} w_i \right) \ln w_i \right] \quad (18)$$

where

$$w_i = \left[\frac{W_i^2 - 4(wx)_i U_i}{W_i^2 - 4(wx)_i U_{i-1}} \right]^{\frac{1}{2}} \left[\frac{W_i - 2(wx)_i^{\frac{1}{2}} U_{i-1}^{\frac{1}{2}}}{W_i - 2(wx)_i^{\frac{1}{2}} U_i^{\frac{1}{2}}} \right] \quad (19)$$

w_i is the coefficient of $(v+\frac{1}{2})^2$

wx_i is the coefficient of $(v+\frac{1}{2})^2$

α_i is the coefficient of $(v+\frac{1}{2}) J(J+1)$ (coupling constant)

B_i is the coefficient of $J(J+1)$

Vanderslice et al. also give a simple interpretation of the $S(\tilde{U}, K)$ function of Klein. $S(\tilde{U}, K)$ is one half the area between the constant total energy curve, \tilde{U} , and the potential curve $V_{\text{eff}}(r)$ (see figure 1).

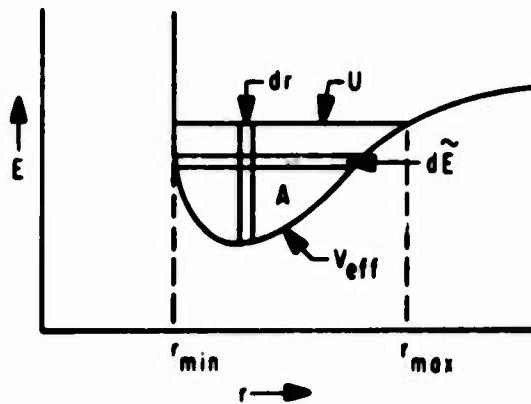


Figure 1. Interpretation of the Klein S Function

Following Vanderslice,

$$dI = \tau dE \quad (20)$$

with

$$\tau = \left(\frac{\mu}{2}\right)^{\frac{1}{2}} \int (E - v_{\text{eff}})^{-\frac{1}{2}} dr \quad (21)$$

putting τdE in for dI in Klein's equation for S ,

$$S(\tilde{U}, K) = \frac{1}{(2\pi^2 \mu)^{\frac{1}{2}}} \int_0^I [\tilde{U} - \tilde{E}(I, K)]^{\frac{1}{2}} dI$$

one finds,

$$S = \frac{1}{2\pi} \int_0^U (\tilde{U} - \tilde{E})^{\frac{1}{2}} \left[(\tilde{E} - \tilde{v}_{\text{eff}})^{-\frac{1}{2}} dr \right] d\tilde{E}$$

or

$$S = \frac{1}{2\pi} dr \int_{V_{\text{eff}}}^U (\tilde{U} - \tilde{E})^{\frac{1}{2}} (\tilde{E} - \tilde{v}_{\text{eff}})^{\frac{1}{2}} d\tilde{E} \quad (22)$$

The lower limit of the second integral is V_{eff} since it is evaluated at a constant value of r .

The last integral becomes, after some manipulation,

$$S = \frac{1}{2} \int_{r_{\min}}^{r_{\max}} dr \int_{V_{\text{eff}}}^U dE = \frac{1}{2} A \quad (23)$$

1. METHODS OF VARIOUS INVESTIGATORS

Many investigators have reported calculating RKR potentials for molecules of importance in heated air. Table 1 contains the name of the investigator (or investigators) and the general method used.

Table 1
INVESTIGATORS USING A WKB-TYPE APPROXIMATION

<u>Name</u>	<u>Method</u>
Flinn, Spindler, Fifer	RKR
Gilmore	RK, KDJ
Ginter, Battino	RKR
Halmann, Laulicht	RK
Jarmain	KDJ
Jain, Shani, Singh	RKR
Krupenie, Weissman	RK
Richards, Barrow	RK-RKR (hybrid)
*Vanderslice et al.	RKR
Zare, Albritton	RK
AFWL	RK

The RK method uses Klein's equations and numerically integrates them in some fashion. The RKR method uses the quadratic fit of Rees in some fashion. The KDJ method makes use of a series developed by Jarmain (Ref. 6) based on a series expansion of a WKB approximation by Dunham (Ref. 7). With some simplifying approximations this expansion is the same as a series expansion of Klein's equations, which are also based on a WKB approximation. Hurley (Ref. 8) has shown the two methods are equivalent and can be deduced from the same basic equation.

2. LIMITATIONS OF RK OR RKR METHODS

Ginter and Battino (Ref. 9) have discussed the effects of experimental errors and errors due to approximations made in the formulation of equations used in the RKR methods on the calculated potential curves. A summary of their conclusions will be presented.

*Co-author with several people on different papers.

The accuracy with which one can represent the vibrational-rotational energy levels of an electronic state of a diatomic molecule by a polynomial $E(v,J)$ primarily determines the accuracy of the calculated potential. The errors in determining $E(v,J)$ fall into three categories:

- (1) Experimental error in spectroscopic data
- (2) Error caused by fitting the best polynomial $E(v,J)$ to the spectroscopic data
- (3) Error caused by fitting the spectroscopic data to a particular form of $E(v,J)$

From (1) there can be errors because of uncertainty in determining B_v^{eff} and ΔG and errors due to using the effective constants directly. From (2) often times the experimental data will fit with any one of several expansions and do it equally well. From (3) if a series of expansions of quadratic form for $E(v,J)$ is assumed, then errors may be introduced because of the fitting of local fluctuations in the experimental data.

3. ZARE PROGRAM AT AFWL

Several years ago R. N. Zare made available to the Air Force Weapons Laboratory (AFWL) a set of computer programs needed to construct R-K molecular potentials for diatomic molecules and to calculate Franck-Condon factors, r-centroids, and relative intensities from these potentials. A summary of the methods of the programs will be given.

The molecular potential generation program is one which was written by J. Kasper (Ref. 10). The equations,

$$f = \frac{h}{2\pi(2\mu)^{\frac{1}{2}}} \int_0^{I'} [U - E(I,K)]^{-\frac{1}{2}} dI \quad (24)$$

$$g = \frac{h}{2\pi(2\mu)^{\frac{1}{2}}} \int_0^{I'} B_v [U - E(I,K)]^{-\frac{1}{2}} dI \quad (25)$$

are integrated directly without assuming an analytic form for the integral near the upper limit.

For the energy $E(I,K)$ of the level of interest either the conventional expansion

$$\begin{aligned} E(v,J) = & \omega_e(v+\frac{1}{2}) - \omega_e x_e(v+\frac{1}{2})^2 + \omega_e y_e(v+\frac{1}{2})^3 \\ & + \omega_e z_e(v+\frac{1}{2})^4 + \omega_e t_e(v+\frac{1}{2})^5 + \dots \\ & + B_v J(J+1) - D_v J^2(J+1)^2 + \dots \end{aligned} \quad (26)$$

or the G_v, B_v obtained directly from the spectroscopic data can be used. The variables I, K are of course related to V, J by

$$I = h(v+\frac{1}{2}) \quad (27)$$

$$K = \frac{\hbar^2}{2\pi^2\mu} J(J+1) \quad (28)$$

From the f, g the values of r_{\min} and r_{\max} are calculated for each vibrational level. These are then used as input data to the Franck-Condon factor program. To calculate the wavefunctions needed in the Franck-Condon factor program, the radial Schrodinger equation is solved (for the wavefunctions) by a numerical method developed by Cooley (Ref. 11). The one-dimensional second order Schrodinger equation,

$$\frac{d^2}{dr^2} \psi + \left[E(v,J) - V_{\text{eff}}(r,J) \right] \psi = 0 \quad (29)$$

where

$E(v,J)$ is the energy of the particular level,

$$V_{\text{eff}}(r,J) = V(r) + \frac{\hbar^2}{8\pi\mu r^2} J(J+1) \quad (30)$$

is the energy of rotationless level corrected for rotation, and ψ , the vibration-rotation wavefunction, is changed to a finite difference equation.

The finite difference equation is solved iteratively for $E(v,J)$ the eigenvalue and ψ the eigenfunction, until the $E(v,J)$ and the previous $E(v,J)$ differ by an arbitrarily small amount. The wavefunctions thus obtained are used in the evaluation of the square of the overlap integral which is the Franck-Condon factor.

$$q_{v'v''} = \int \psi_{v'J'} \psi_{v''J''} dr^2 \quad (31)$$

They are also used in evaluating the r-centroids.

$$r_{v'v''} = \frac{\int \psi_{v'} r \psi_{v''} dr}{\int \psi_{v'} \psi_{v''} dr} \quad (32)$$

$$r_{v'v''}^2 = \frac{\int \psi_{v'} r^2 \psi_{v''} dr}{\int \psi_{v'} \psi_{v''} dr} \quad (33)$$

The integrals are all evaluated using a Simpson's rule numerical integration procedure. The relative intensities scaled to ten are also calculated.

The programs provided by Dr. Zare have been adapted for use on the AFWL CDC 6600 computer. Since this computer carries 15 decimal numbers per word, the double precision subroutines were removed. The (v',v'') array size for the computed Franck-Condon factor was increased to (20,23). Some of the input statements were modified and output statements were added. Aside from these changes the program used at AFWL is the same as the one developed and used by Dr. Zare.

SECTION II
MOLECULAR BAND SYSTEMS CONSIDERED

The motivation for calculating Franck-Condon factors at AFWL is their use in calculating transition strengths of diatomic molecules. These strengths are used in part to calculate absorption coefficients which in turn are frequency averaged over prechosen frequency groups to give opacities for air. These opacities are desired over a large temperature density range. When determining which molecules are candidates for inclusion in the opacity calculation, one must take into account the chemistry that goes on in this heated air. After picking the potential molecules one looks at the various transitions allowed in the molecules and the relative strengths and positions (in energy) of the transitions. Then from these one arrives at a list of important electronic band systems of diatomic molecules in heated air.

The following table contains information on all transitions considered in the present work. The transition involved, common name of the band system, the source of the potential, and array size calculated are listed.

Table 2
TRANSITIONS INCLUDED

<u>States involved</u>	<u>Name</u>	<u>Source of potential</u>		<u>Array size</u> (v'v")
		<u>State</u> <u>Upper</u>	<u>Lower</u>	
CN $B^2\Sigma^+$ -CN $X^2\Sigma^+$	CN violet	13	13	(18,18)
CN $A^2\pi_{1/2}$ -CN $X^2\Sigma^+$	CN red	13	13	(18,18)
CN $A^2\pi_{3/2}$ -CN $X^2\Sigma^+$	CN red	13	13	(18,18)
CO $A^1\pi$ -CO $X^1\Sigma^+$	CO 4th positive	16	16	(20,24)
$N_2 B^3\pi_g$ - $N_2 A^3\Sigma_u^+$	1st positive	18	18	(17,13)
$N_2 C^3\pi_u$ - $N_2 B^3\pi_g$	2nd positive	18	18	(4,17)
$N_2 b'^1\Sigma_u^+$ - $N_2 X^1\Sigma_g^+$	Birge-Hopfield #1	33	19	(20,21)
$N_2 b'^1\Sigma_u$ - $N_2 X^1\Sigma_g$	Birge-Hopfield #2	33	19	(24,21)

Table 2 (cont'd)

<u>States involved</u>	<u>Name</u>	<u>Source of potential State</u>		<u>Array size (v'v")</u>
		<u>Upper</u>	<u>Lower</u>	
$N_2^+ A^2\pi_u^- - N_2^+ X^2\Sigma_g^+$	Meinel	33	33	(20,20)
$N_2^+ B^2\Sigma_u^+ - N_2^+ X^2\Sigma_g^+$	1st negative	33	33	(20,20)
$N_2^+ C^2\Sigma_u^+ - N_2^+ X^2\Sigma_g^+$	2nd negative	33	33	(10,20)
$NO A^2\Sigma^+ - NO X^2\pi_{1/2}$	γ (gamma)	22	23	(5,23)
$NO A^2\Sigma^+ - NO X^2\pi_{3/2}$	γ (gamma)	22	23	(5,23)
$NO B^2\pi - NO X^2\pi_{1/2}$	β (beta)	22	23	(19,23)
$NO B^2\pi - NO X^2\pi_{3/2}$	β (beta)	22	23	(19,23)
$NO C^2\pi - NO X^2\pi_{1/2}$	δ (delta)	22	23	(4,23)
$NO C^2\pi - NO X^2\pi_{3/2}$	δ (delta)	22	23	(4,23)
$NO D^2\Sigma^+ - NO X^2\pi_{1/2}$	ϵ (epsilon)	33	23	(7,23)
$NO D^2\Sigma^+ - NO X^2\pi_{3/2}$	ϵ (epsilon)	33	23	(7,23)
$NO B'^2\Delta_1^- - NO X^2\pi_{1/2}$	β' (beta prime)	22	23	(5,23)
$NO B'^2\Delta_1^- - NO X^2\pi_{3/2}$	β' (beta prime)	22	23	(5,23)
$NO E^2\Sigma^+ - NO X^2\pi_{1/2}$	γ' (gamma prime)	22	23	(5,23)
$NO E^2\Sigma^+ - NO X^2\pi_{3/2}$	γ' (gamma prime)	22		(5,23)
$NO G^2\Sigma - NO X^2\pi_{1/2}$	Lagergmist-Miescher	33	23	(7,23)
$NO C^2\pi - NO A^2\Sigma^+$	Heath	22	22	(4,5)
$NO D^2\Sigma^+ - NO A^2\Sigma^+$	Feast 1	22	22	(7,5)
$NO E^2\Sigma^+ - NO A^2\Sigma^+$	Feast 2	22	22	(5,5)
$NO E^2\Sigma^+ - NO C^2\pi$		22	22	(5,4)
$NO E^2\Sigma^+ - NO D^2\Sigma^+$	Feast-Heath	22	33	(5,7)
$O_2 B^3\Sigma_u^- - O_2 X^3\Sigma_g^-$	Schumann-Runge	33	33	(20,23)
	$N_2 - N_2^+$			
$N_2 X^1\Sigma_g^+ - N_2^+ X^2\Sigma_g^+$	1st	33	33	(20,20)

Table 2 (cont'd)

<u>States involved</u>	<u>Name</u>	<u>Source of potential</u>		<u>Array size (v'v")</u>
		<u>State</u>	<u>Upper Lower</u>	
$N_2 X^1\Sigma^+_g - N_2^+ A^2\pi_u$	2nd		33 33	(20,20)
$N_2 X^1\Sigma^+_g - N_2^+ B^2\Sigma^+_u$	3rd		33 33	(20,20)
$N_2 X^1\Sigma^+_g - N_2^+ C^2\Sigma^+_u$	4th		33 33	(10,20)
	$O_2 - O_2^+$			
$O_2 X^3\Sigma^-_g - O_2^+ X^2\pi_g$	1st		33 33	(14,23)
$O_2 X^3\Sigma^-_g - O_2^+ a^4\pi_u$	2nd		33 33	(10,23)
$O_2 X^3\Sigma^-_g - O_2^+ A^2\pi_u$	3rd		33 33	(10,23)
$O_2 X^3\Sigma^-_g - O_2^+ b^4\Sigma^-_g$	4th		33 33	(10,23)
$O_2 X^3\Sigma^-_g - O_2^+ 2\Sigma^-_g$	5th		33 33	(10,23)
$O_2 X^3\Sigma^-_g - O_2^+ c^4\Sigma^-_u$	6th		33 33	(10,23)

1. CN (CYANOGEN) BAND SYSTEMS

The potentials used to calculate Franck-Condon factors were taken from the paper by Fallon, Vanderslice, and Cloney (Ref. 13). Tables 3 through 6 contain the data for the potential energy curves for the various CN states used. Table 7 contains other molecular data needed by the FRANKON program.

Table 3*

POTENTIAL ENERGY FOR THE CN $X^2\Sigma^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1031.1	1.1237	1.2244	0.1278
1	3073.6	1.0923	1.1676	0.3811
2	5089.7	1.0722	1.2997	0.6310
3	7079.5	1.0566	1.3274	0.8777
4	9042.8	1.0438	1.3525	1.1211
5	10980.0	1.0327	1.3760	1.3613
6	12890.0	1.0230	1.3984	1.5981

Table 3* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
7	14775.0	1.0143	1.4198	1.8317
8	16632.0	1.0063	1.4406	2.0620
9	18463.0	0.9991	1.4610	2.2890
10	20267.0	0.9924	1.4809	2.5127
11	22045.0	0.9861	1.5005	2.7330
12	23797.0	0.9803	1.5200	2.0503
13	25520.0	0.9749	1.5393	3.1639
14	27217.0	0.9696	1.5583	3.3743
15	28887.0	0.9648	1.5774	3.5813
16	30530.0	0.9602	1.5964	3.7850
17	32146.0	0.9558	1.6153	3.9853
18	33734.0	0.9516	1.6343	4.1823

*Reference 13.

Table 4*

POTENTIAL ENERGY FOR THE CN A²π_{3/2} STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	903.99	1.1827	1.2900	0.1121
1	2691.1	1.1482	1.3354	0.3336
2	4452.9	1.1269	1.3701	0.5521
3	6189.4	1.1105	1.4001	0.7673
4	7900.4	1.0969	1.4273	0.9795
5	9585.0	1.0852	1.4529	1.1884
6	11245.0	1.0749	1.4773	1.3942
7	12880.0	1.0657	1.5007	1.5968

Table 4* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
8	14487.0	1.0573	1.5236	1.7960
9	16070.0	1.0477	1.5459	1.9923
10	17627.0	1.0526	1.5679	2.1853
11	19158.0	1.0360	1.5896	2.3751
12	20663.0	1.0298	1.6111	2.5617
13	22142.0	1.0240	1.6325	2.7451
14	23594.0	1.0186	1.6538	2.9254
15	25021.0	1.0134	1.6750	3.1020
16	26422.0	1.0083	1.6960	3.2757
17	27795.0	1.0038	1.7175	3.4460
18	29142.0	0.9994	1.7388	3.6130

*Reference 13.

Table 5*

POTENTIAL ENERGY FOR THE CN A²π_{1/2} STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	903.99	1.1816	1.2891	0.1121
1	2691.1	1.1484	1.3356	0.3336
2	4452.9	1.1272	1.3704	0.5521
3	6189.4	1.1109	1.4006	0.7673
4	7900.4	1.0975	1.4280	0.9795
5	9585.9	1.0860	1.4527	1.1884
6	11245.0	1.0759	1.4783	1.3942
7	12880.0	1.0668	1.5019	1.5968
8	14487.0	1.0587	1.5249	1.7960
9	16070.0	1.0512	1.5475	1.9923

Table 5* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
10	17627.0	1.0443	1.5696	2.1853
11	19158.0	1.0379	1.4916	2.3751
12	20663.0	1.0319	1.6133	2.5617
13	22142.0	1.0263	1.6348	2.7451
14	23594.0	1.0211	1.6563	2.9254
15	25021.0	1.0161	1.6778	3.1020
16	26422.0	1.0115	1.6992	3.2757
17	27795.0	1.0070	1.7207	3.4460
18	29142.0	1.0028	1.7423	3.6130

*Reference 13.

Table 6*

POTENTIAL ENERGY FOR THE CN B²Σ⁺ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1077.0	1.104	1.203	0.1335
1	3200.0	1.074	1.246	0.3968
2	5284.0	1.055	1.279	0.6551
3	7325.0	1.040	1.307	0.9081
4	9321.0	1.027	1.333	1.1556
5	11269.0	1.016	1.358	1.3971
6	13167.0	1.007	1.383	1.6324
7	15011.0	0.999	1.407	1.8611
8	16799.0	0.992	1.432	2.0827
9	18527.0	0.986	1.457	2.2969
10	20192.0	0.980	1.483	2.5034

Table 6* (cont'd)

<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>v(ev)</u>
11	21795.0	0.974	1.509	2.7021
12	23338.0	0.970	1.535	2.8933
13	24821.0	0.965	1.562	3.0773
14	26249.0	0.961	1.589	3.2542
15	27623.0	0.957	1.617	3.4247
16	28948.0	0.953	1.644	3.5889
17	30228.0	0.950	1.672	3.7475
18	31464.0	0.946	1.701	3.9008

*Reference 13.

Table 7

ADDITIONAL DATA NEEDED FOR THE CN MOLECULE

<u>State</u>	<u>De</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>Te</u>
X ² Σ^+	61525.88	1.8996	0.01735	0	0.0
A ² $\pi_{3/2}$	52279.86	1.7165	0.01746	0	9222.04
A ² $\pi_{1/2}$	52279.86	1.7165	0.01746	0	9272.62
B ² Σ^+	54774.34	1.9701	0.02215	0	25752.4

2. CO (CARBON MONOXIDE) BAND SYSTEMS

The only band of CO considered to be of possible importance in absorption in heated air is the CO 4th positive system. The potentials used in calculating the Franck-Condon factors were taken from the paper by Krupenie and Weisman (Ref. 16). Tables 8 and 9 contain the data for the potential curves of the lower and upper states. Table 10 contains other molecular data needed by the program.

Table 8*

POTENTIAL ENERGY FOR THE CO $X^1\Sigma^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1081.590	1.083	1.179	0.1341
1	3224.864	1.053	1.220	0.3998
2	5341.654	1.034	1.250	0.6623
3	7432.026	1.020	1.276	0.9214
4	9496.948	1.008	1.300	1.1773
5	11533.76	0.997	1.322	1.4300
6	13545.20	0.988	1.343	1.6794
7	15530.64	0.980	1.363	1.9255
8	17489.9	0.972	1.383	2.1684
9	19423.5	0.965	1.402	2.4081
10	21330.7	0.959	1.420	2.6446
11	23212.4	0.953	1.438	2.8779
12	25068.5	0.947	1.456	3.1080
13	26898.4	0.942	1.474	3.3349
14	28703.2	0.937	1.492	3.5587
15	30482.7	0.932	1.509	3.7793
16	32235.4	0.928	1.526	3.9966
17	33963.9	0.923	1.544	4.2109
18	35666.8	0.919	1.561	4.4220
19	37344.4	0.916	1.579	4.6300
20	38997.5	0.912	1.596	4.9349
21	40625.7	0.908	1.614	5.0368
22	42208.0	0.905	1.631	5.2330
23	43776.0	0.901	1.649	5.4274

*Reference 16.

Table 9*

POTENTIAL ENERGY FOR THE CO A²₁ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	753.49	1.183	1.297	0.0934
1	2242.3	1.148	1.348	0.2780
2	3685.1	1.126	1.387	0.4569
3	5097.9	1.110	1.422	0.6320
4	6476.1	1.096	1.454	0.8029
5	7818.2	1.085	1.484	0.9693
6	9125.0	1.075	1.514	1.1313
7	10401.8	1.066	1.542	1.2896
8	11641.0	1.058	1.571	1.4433
9	12846.9	1.051	1.599	1.5928
10	14018.8	1.044	1.627	1.7381
11	15155.6	1.038	1.656	1.8790
12	16262.0	1.031	1.685	2.0162
13	17333.0	1.027	1.714	2.1490
14	18371.0	1.022	1.743	2.2777
15	19366.0	1.017	1.773	2.4010
16	20330.0	1.013	1.804	2.5205
17	21257.0	1.009	1.837	2.6355
18	22380.0	1.005	1.871	2.7447
19	22970.0	1.001	1.090	2.8478
20	23762.0	0.996	1.051	2.9460

*Reference 16.

Table 10*

ADDITIONAL DATA NEEDED FOR THE CO MOLECULE

($\nu = 6.85841$)

<u>State</u>	<u>D_e</u>	<u>B_e</u>	<u>α_e</u>	<u>γ_e</u>	<u>T_e</u>
X ¹ Σ^+	89597.4	1.93127	0.617513	2.960E-6	0.0
A ¹ π	24522.8	1.226	0.018	0.0	133740.0

*Gilmore, DASA Handbook 1917 old copy Volume I tables.

3. N₂ (NITROGEN) BAND SYSTEMS

The potentials used to calculate the Franck-Condon factors for the nitrogen systems came from several sources. The X¹ Σ_g^+ , A³ Σ_u^+ , B³ π_u , and C³ π_u states contained in tables 11 through 14 were taken from the paper by Benesch et al. (Ref. 18). The potentials used for the b¹ π_u and b'¹ Σ_u^+ states were generated at AFWL with program TURNGPT and are listed in tables 15 and 16, respectively. The data for the b¹ π_u state are from Lofthus (Ref. 19) and the data for the b'¹ Σ_u^+ state are from Wilkinson (Ref. 20). These data are listed in tables 17 through 18.

Table 11*

POTENTIAL ENERGY FOR THE N₂ X¹ Σ_g^+ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>V(ev)</u>
0	1175.5	1.055 ₀	1.145 ₆	0.14573
1	3505.2	1.026 ₆	1.184 ₃	0.42456
2	5806.5	1.008 ₃	1.213 ₀	0.71987
3	8079.2	0.994 ₂	1.237 ₇	1.00163
4	10323.3	0.982 ₆	1.260 ₀	1.27985
5	12538.8	0.972 ₅	1.280 ₉	1.55452
6	14725.4	0.963 ₆	1.300 ₇	1.82561

Table 11* (cont'd)

<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>v(ev)</u>
7	16883.1	0.955 ₆	1.319 ₇	2.09311
8	19011.8	0.948 ₄	1.338 ₂	2.35702
9	21111.5	0.941 ₇	1.356 ₁	2.61733
10	23182.0	0.935 ₅	1.373 ₈	2.87403
11	25223.3	0.929 ₈	1.391 ₁	3.12710
12	27235.3	0.924 ₄	1.408 ₂	3.37654
13	29218.0	0.919 ₄	1.425 ₂	3.62235
14	31171.2	0.914 ₆	1.442 ₀	3.86450
15	33094.9	0.910 ₁	1.458 ₈	4.10300
16	34989.0	0.905 ₈	1.475 ₅	4.33782
17	36853.5	0.901 ₇	1.492 ₁	4.56898
18	38688.3	0.897 ₈	1.508 ₈	4.79645
19	40493.4	0.894 ₀	1.525 ₅	5.02024
20	42268.6	0.890 ₄	1.542 ₃	5.24032
21	44014.1	0.887 ₀	1.559 ₁	5.45672

*Reference 18.

Table 12*

POTENTIAL ENERGY FOR THE N ₂ A ^{3Σ_u⁺} STATE				
<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>v(ev)</u>
0	726.80	1.2329	1.3482	0.0901
1	2159.67	1.1979	1.3992	0.2678
2	3564.87	1.1758	1.4378	0.4420
3	4942.36	1.1589	1.4715	0.6127
4	6292.03	1.1450	1.5025	0.7801
5	7613.75	1.1332	1.5319	0.9439

Table 12* (cont'd)

<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>v(ev)</u>
6	8907.33	1.1229	1.5602	1.1043
7	10172.54	1.1138	1.5877	1.2612
8	11409.10	1.1055	1.6149	1.4145
9	12616.69	1.0980	1.6417	1.5642
10	13794.95	1.091 ₁	1.668 ₅	1.7103
11	14943.47	1.084 ₇	1.695 ₃	1.8526
12	16061.80	1.078 ₇	1.722 ₂	1.9913
13	17149.44	1.073 ₂	1.749 ₃	2.1261

*Reference 18.

Table 13*

POTENTIAL ENERGY FOR THE N ₂ B ^{3π} _g STATE				
<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>v(ev)</u>
0	863.16	1.1631	1.2689	0.10702
1	2568.14	1.1306	1.3150	0.31840
2	4244.46	1.1099	1.3497	0.52623
3	5891.92	1.0940	1.3798	0.73049
4	7510.38	1.0809	1.4074	0.93114
5	9099.74	1.0697	1.4334	1.12819
6	10659.92	1.0599	1.4583	1.32163
7	12190.86	1.0511	1.4825	1.51144
8	13692.50	1.0432	1.5061	1.69761
9	15164.76	1.0360	1.5294	1.88014
10	16607.54	1.0294	1.5524	2.05902
11	18020.70	1.0233	1.5753	2.23422
12	19404.04	1.0176	1.5981	2.40573

Table 13* (cont'd)

<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>V(ev)</u>
13	20757.31	1.012 ₃	1.621 ₀	2.57351
14	22080.16	1.007 ₄	1.644 ₀	2.73752
15	23372.16	1.002 ₇	1.667 ₂	2.89770
16	24632.76	0.998 ₂	1.690 ₆	3.05399
17	25861.32	0.994 ₀	1.714 ₃	3.20631

*Reference 18.

Table 14*

POTENTIAL ENERGY FOR THE N ₂ C ³ π _u STATE				
<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{min}(Å)</u>	<u>r_{max}(Å)</u>	<u>V(ev)</u>
0	1016.71	1.1030	1.2005	0.12605
1	3011.11	1.0730	1.2438	0.37332
2	4951.90	1.0540	1.2771	0.61394
3	6825.93	1.0395	1.3076	0.84629
4	8607.21	1.0282	1.3388	1.06713

*Reference 18.

Table 15*

POTENTIAL ENERGY OF THE N ₂ b ¹ π _u STATE				
<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	412.5	1.23007	1.38773	0.0511
1	1114.5	1.16992	1.45950	0.1381
2	1779.5	1.13007	1.51097	0.2206
3	2407.5	1.09562	1.55852	0.2984
4	2992.5	1.06450	1.60407	0.3710

Table 15* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
5	3546.5	1.03665	1.64718	0.4396
6	4062.5	1.00840	1.69329	0.5036
7	4542.4	0.98508	1.73570	0.5631

*From TURNGPT using Lofthus data.

Table 16*

POTENTIAL ENERGY OF THE N₂ b' $^1\Sigma_u^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	374.6	1.36740	1.52792	0.0464
1	1116.6	1.31442	1.59394	0.1384
2	1848.9	1.38936	1.65220	0.2292
3	2571.6	1.25162	1.68331	0.3188
4	3284.7	1.22812	1.72036	0.4072
5	3988.2	1.20746	1.75474	0.4944
6	4682.0	1.18887	1.78724	0.5804

*From TURNGPT using Wilkinson data.

Table 17

ADDITIONAL DATA NEEDED FOR THE N₂ MOLECULE

<u>State</u>	<u>D_e</u>	<u>B_e</u>	<u>a_e</u>	<u>y_e</u>	<u>T_e</u>
X ¹ Σ_g^+	78717.0	1.9987	0.0178	0.0	0.0
A ³ Σ_u^+	28499.0	1.4545	0.01794	-9.2 x 10 ⁻⁵	50218.0
B ³ π_u	38306.0	1.6375	0.01794	-7.4 x 10 ⁻⁵	59639.0
C ³ π_u	28643.0	1.8259	0.0197	0.0	69302.0

Table 17 (cont'd)

<u>State</u>	<u>De</u>	<u>Be</u>	<u>ae</u>	<u>Ye</u>	<u>Te</u>
$b^1\pi_u$	55655.0*	1.154	0.0048	0.0	104473.0
$b'^1\Sigma_u^+$	55655.0*	---	---	---	102288.0

*Estimated value.

Table 18

MOLECULAR DATA NEEDED FOR TURNGPT ($N_2 b'^1\Sigma_u^+$)

<u>State</u>	<u>We</u>	<u>Wexe</u>	<u>Weye</u>	<u>Weze</u>	<u>Be</u>	<u>ae</u>	<u>Ye</u>	<u>re</u>
$b'^1\Sigma_u^+$	751.64	4.82	0	0	1.154	0.0048	0	1.4443

Table 19

MOLECULAR DATA NEEDED FOR TURNGPT ($N_2 b^1\pi_u$)

<u>v</u>	<u>Gv</u>	<u>Bv</u>
0	0	1.41
1	702	1.41
2	1367	1.40
3	1995	1.41
4	2580	1.48
5	3134	1.47
6	3650	---

4. N_2^+ (NITROGEN MOLECULAR ION) BAND SYSTEMS

The potentials used to generate the Franck-Condon factors for the N_2^+ band systems were calculated with program TURNGPT. The $A^2\pi_u$ and $C^2\Sigma_u^+$ states were generated using spectroscopic constants given by Gilmore (Ref. 21). These are given in table 24. The $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$ states were generated by using spectroscopic data from Lofthus (Ref. 19). These data are listed in tables 25 and 26.

The B_v for the missing levels was obtained by graphical interpolation. The

generated potentials are listed in tables 20 through 23.

Table 20*

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	1099.4	1.07794	1.1664
1	3274.2	1.04341	1.20672
2	5416.4	1.02546	1.23763
3	7525.8	1.01122	1.26388
4	9602.2	0.99944	1.28783
5	11645.4	0.97947	1.20991
6	13654.4	0.97947	1.33082
7	15630.1	0.97184	1.35192
8	17570.0	0.96441	1.37203
9	19477.0	0.95803	1.39205
10	21349.0	0.95185	1.41160
11	23185.9	0.94604	1.43092
12	24987.0	0.94066	1.45022
13	26751.8	0.93552	1.46943
14	28479.9	0.93092	1.48894
15	30171.0	0.92638	1.50835
16	31824.5	0.92239	1.52823
17	33439.9	0.91853	1.54825
18	35016.7	0.91482	1.56848
19	36554.0	0.91152	1.58931
20	38051.7	0.90810	1.61014

*From Lofthus data.

Table 21*

POTENTIAL ENERGY FOR THE $N_2^+ A^2\pi_u$ STATE				
<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	947.96	1.02650	1.22743	0.1175
1	2821.38	1.09570	1.27158	0.3498
2	4664.80	1.07615	1.30488	0.5783
3	6478.22	1.06118	1.33368	0.8031
4	8271.64	1.04887	1.38479	1.0242
5	10015.06	1.03838	1.38479	1.2416
6	11738.48	1.02917	1.40847	1.4553
7	13431.90	1.02097	1.43137	1.6652
8	15095.32	1.01357	1.45371	1.8714
9	16728.74	1.00681	1.47563	2.0739
10	18332.16	1.00061	1.40726	2.2727
11	19905.58	0.99487	1.51867	2.4678
12	21449.00	0.98954	1.53995	2.6791
13	22962.42	0.98455	1.56116	2.8468
14	24445.84	0.97987	1.58235	3.0307
15	25897.26	0.97546	1.60356	3.2109
16	27322.68	0.97130	1.62484	3.3880
17	28716.10	0.967356	1.64622	2.5601
18	30079.52	0.96361	1.66774	3.7291
19	31412.94	0.96003	1.68943	3.8944
20	32716.36	0.95662	1.71132	4.0560

*From Gilmore's constants.

Table 22*

POTENTIAL ENERGY FOR THE $N_2^+ B^2\Sigma_u^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1197.15	1.03331	1.12304	0.1484
1	3588.66	1.00546	1.16196	0.4424
2	5887.46	0.98795	1.19199	0.7299
3	9147.86	0.97409	1.21811	1.0101
4	10344.26	0.96323	1.24330	1.2824
5	12467.06	0.95501	1.26903	1.5456
6	14508.06	0.94720	1.27401	1.7986
7	16459.16	0.94043	1.32000	2.0405
8	18291.36	0.93404	1.34765	2.2677
9	20018.26	0.92856	1.37643	2.4818
10	21614.96	0.92315	1.40798	2.6797
11	23094.86	0.91867	1.44118	2.8632
12	24466.26	0.91496	1.117632	3.0332
13	25742.56	0.91145	1.51208	3.1914
14	26938.86	0.90846	1.54832	3.3397
15	28065.46	0.90544	1.58452	3.4794
16	29132.56	0.90303	1.62095	3.6117
17	30148.06	0.90104	1.65763	3.7376
18	31114.06	0.89893	1.69439	3.8574
19	32036.06	0.89687	1.73160	3.9717
20	32858.06	0.89012	1.78474	4.0736

*From Lofthus data.

Table 23*

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1034.08	1.21465	1.31124	0.1282
1	3085.06	1.18158	1.34967	0.3824
2	5111.94	1.15962	1.37772	0.6337
3	7113.28	1.14238	1.40182	0.8818
4	9087.64	1.12798	1.42383	1.1266
5	11033.58	1.11558	1.44462	1.3679
6	12949.66	1.10471	1.46470	1.6054
7	14832.44	1.09508	1.48437	1.8391
8	16686.48	1.08646	1.50386	2.0687
9	18504.34	1.07874	1.52333	2.2941
10	20286.58	1.07182	1.54294	2.5150

*From Gilmore's constants

Table 24

ADDITIONAL DATA NEEDED FOR THE N₂⁺ MOLECULE

<u>State</u>	<u>We</u>	<u>W_{exe}</u>	<u>W_{e ye}</u>	<u>W_{e ze}</u>	<u>W_{e Te}</u>	<u>Te</u>
X ² Σ _g ⁺	2207.17	16.146	-2.85 x 10 ⁻²	9.2 x 10 ⁻⁴	0	0.0
A ² π _u ⁺	1903.42	15.0	0.0	0.0	0	8219.6
B ² Σ _u ⁺	2418.7	22.53	-6.70 x 10 ⁻¹	4.0 x 10 ⁻²	0	25461.6
C ² π _u ⁺	2073	10.97	-2.40 x 10 ⁻¹	0.0	0	64607.5

<u>State</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>de</u>	<u>re</u>
X ² Σ _g ⁺	1.9258	0.01743	-1.64 x 10 ⁻⁴	0	1.118
A ² π _u ⁺	1.748	0.02	0.00	0	1.117
B ² Σ _u ⁺	2.083	0.0183	-1.65 x 10 ⁻³	0	1.075
C ² π _u ⁺	1.5124	0.0017	-7.50 x 10 ⁻⁴	0	1.262

Table 25
MOLECULAR DATA NEEDED FOR TURNGPT $\left(\text{N}_2^+ \text{ X}^2\Sigma_g^+\right)$

<u>v</u>	<u>G_v</u>	<u>B_v</u>
0	1099.4	1.922
1	3274.2	1.902
2	5416.4	1.879
3	7525.8	1.861
4	9602.2	1.841
5	11645.2	1.826
6	13654.4	1.808
7	15630.1	1.781
8	17570.0	1.766
9	19477.0	1.740
10	21349.1	1.724
11	23185.9	1.703
12	24987.0	1.683
13	26751.8	1.663
14	28479.9	1.639
15	30171.0	1.620
16	31824.5	1.593
17	33439.9	1.572
18	35016.7	1.548
19	36554.0	1.522
20	38051.7	1.500

Table 26

MOLECULAR DATA NEEDED FOR TURNGPT $N_2^+ B^2\Sigma_u^+$

<u>v</u>	<u>Gv</u>	<u>Bv</u>
0	1197.16	2.073
1	3568.66	2.049
2	5887.46	2.025
3	8147.86	2.002
4	10344.26	1.968
5	12467.06	1.926
6	14508.06	1.896
7	16459.16	1.896
8	18291.36	1.81
9	20018.26	1.761
10	21614.06	1.710
11	23094.86	1.653
12	24466.26	1.595
13	25742.56	1.545
14	26938.86	1.494
15	28065.46	1.452
16	29132.56	1.404
17	30148.06	1.361
18	31114.06	1.323
19	32036.06	1.285
20	32858.06	1.250

5. NO (NITRIC OXIDE) BAND SYSTEMS

The molecular potentials used to calculate the various NO band system Franck-Condon factors came from three sources. The $X^2\pi_{1/2}$, $X^2\pi_{3/2}$ states were from Vanderslice (Ref. 23). The $A^2\Sigma^+$, $B^2\pi$, $C^2\pi$, $B'^2\Delta$, $E^2\Sigma^+$ states were from Vanderslice et al. (Ref. 22). The NO $D^2\Sigma^+$ state potential was generated with program TURNGPT using molecular constants from Gilmore (Ref. 21). The potentials are listed in tables 27 through 34. The spectroscopic constants used to generate the D state potential are listed in table 35.

Table 27*

POTENTIAL ENERGY FOR THE NO $X^2\pi_{1/2}$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	948.5	1.202	1.105	0.1176
1	2825.0	1.245	1.074	0.3503
2	4673.0	1.276	1.055	0.5795
3	6493.0	1.304	1.041	0.8051
4	8285.0	1.329	1.028	1.027
5	10048.0	1.352	1.018	1.246
6	11784.0	1.375	1.009	1.461
7	13492.0	1.396	1.000	1.673
8	15172.0	1.417	0.993	1.881
9	16824.0	1.438	0.986	2.086
10	18448.0	1.458	0.974	2.388
11	20044.0	1.478	0.980	2.485
12	21613.0	1.497	0.974	2.680
13	23152.0	1.517	0.968	2.871
14	24665.0	1.537	0.963	3.058
15	26149.0	1.556	0.958	3.131
16	27605.0	1.576	0.954	3.423
17	29034.0	1.596	0.945	3.600

Table 27* (cont'd)

<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
18	30434.0	1.615	0.941	3.774
19	31805.0	1.636	0.937	3.944
20	33141.0	1.656	0.934	4.109
21	34443.0	1.677	0.930	4.271
22	35714.0	1.698	0.926	4.418
23	36953.0	1.719	0.923	4.582

*Reference 23.

Table 28*

POTENTIAL ENERGY FOR THE NO X²π_{3/2} STATE

<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	948.5	1.204	1.106	0.1176
1	2825.0	1.246	1.076	0.3503
2	4673.0	1.278	1.057	0.5795
3	6493.0	1.305	1.042	0.8051
4	8285.0	1.330	1.030	1.027
5	10048.0	1.354	1.019	1.246
6	11784.0	1.376	1.010	1.461
7	13492.0	1.397	1.002	1.673
8	15172.0	1.418	0.994	1.881
9	16824.0	1.439	0.987	2.086
10	18448.0	1.459	0.981	2.288
11	20044.0	1.479	0.975	2.485
12	21613.0	1.499	0.969	2.680
13	23152.0	1.518	0.964	2.871

Table 28* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
14	24663.0	1.538	0.959	3.058
15	26145.0	1.558	0.955	3.242
16	27599.0	1.577	0.950	3.422
17	29024.0	1.597	0.946	3.599
18	30423.0	1.617	0.942	3.772
19	31790.0	1.637	0.938	3.942
20	33124.0	1.657	0.934	4.107
21	34424.0	1.678	0.930	4.269
22	35695.0	1.698	0.926	4.426
23	36938.0	1.719	0.923	4.580

*Reference 23.

Table 29*

POTENTIAL ENERGY FOR THE NO A²Σ⁺ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	1183.0	1.109	1.022	0.1467
1	3525.0	1.147	0.995	0.4371
2	5835.0	1.175	0.977	0.7235
3	8111.0	1.199	0.964	1.006
4	10354.0	1.220	0.953	1.284
5	12564.0	1.242	0.943	1.558

*Reference 23.

Table 30*

POTENTIAL ENERGY OF THE NO $B^2\pi$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	516.8	1.488	1.356	0.0641
1	1540.0	1.545	1.315	0.191
2	2549.0	1.588	1.289	0.316
3	3545.0	1.625	1.269	0.440
4	4519.0	1.658	1.253	0.560
5	5492.0	1.690	1.239	0.681
6	6447.0	1.719	1.226	0.799
7	7390.0	1.748	1.215	0.917
8	8323.0	1.776	1.205	1.032
9	9238.0	1.804	1.196	1.146
10	10144.0	1.831	1.188	1.258
11	11030.0	1.857	1.180	1.368
12	11911.0	1.883	1.173	1.477
13	12772.0	1.909	1.167	1.584
14	13609.0	1.935	1.161	1.688
15	14463.0	1.962	1.154	1.793
16	15293.0	1.989	1.147	1.896
17	16081.0	2.015	1.142	1.994
18	16859.0	2.041	1.136	2.091
19	17612.0	2.068	1.130	2.184

*Reference 23.

Table 31*

POTENTIAL ENERGY OF THE NO C² π STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	1194.0	1.109	1.022	0.1481
1	3556.0	1.148	0.997	0.4409
2	5922.0	1.178	0.981	0.7343
3	8192.0	1.204	0.970	1.016
4	10491.0	1.228	0.961	1.301

*Reference 23.

Table 32*

POTENTIAL ENERGY OF THE NO B'² Δ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	604.0	1.368	1.246	0.07493
1	1789.0	1.424	1.209	0.2219
2	2943.0	1.466	1.186	0.3649
3	4062.0	1.503	1.168	0.5037
4	5177.0	1.539	1.153	0.6420
5	6212.0	1.570	1.139	0.7703

*Reference 23.

Table 33*

POTENTIAL ENERGY OF NO $E^2\Sigma^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{max}(Å)</u>	<u>r_{min}(Å)</u>	<u>V(ev)</u>
0	1183.0	1.112	1.025	0.1467
1	3525.0	1.150	0.997	0.4371
2	5835.0	1.177	0.980	0.7235
3	8114.0	1.202	0.966	1.006
4	10360.0	1.223	0.955	1.285
5	12575.0	1.244	0.945	1.559

*Reference 23.

Table 34*

POTENTIAL ENERGY FOR THE NO $D^2\Sigma^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1156.336	1.02039	1.10891	0.1433
1	3438.004	0.99320	1.14762	0.4262
2	5687.031	0.97601	1.17645	0.7050
3	7918.479	0.97601	1.20099	0.9817
4	10152.686	0.96318	1.22264	1.2586
5	12415.274	0.94545	1.24187	1.5392
6	14737.141	0.93970	1.25881	1.8270
7	17154.469	0.93579	1.27350	2.1267

*From TURNGPT using Gilmore's constants

Table 35
MOLECULAR DATA NEEDED FOR TURNGPT (NO D² Σ)

<u>We</u>	<u>W_{xe}</u>	<u>W_{ye}</u>	<u>W_{ze}</u>	<u>B_e</u>	<u>a_e</u>	<u>y_e</u>	<u>r_e</u>
2323.9	22.885	0.75	0.22	2.0026	2.175×10^{-2}	0	1.062

6. O₂ (OXYGEN) BAND SYSTEM

Franck-Condon factors were calculated for only the O₂ Schumann-Runge band system. The potentials needed, O₂ X³ Σ and O₂ B³ Σ , were calculated with program TURNGPT using data from Wallace (Ref. 24). The G, ΔG , B_v were each plotted and the best smooth curve was drawn through these. These smoothed values were then used as input data to TURNGPT. The B³ Σ state was found to have a hook near the dissociation limit on the inner branch of the potential curve. This is similar to the findings of many other investigators, for example, Vanderslice et al. (Ref. 25), F. Gilmore (Ref. 26), Richards and Barrow (Ref. 27), *Ginter, Battino (Ref. 28).

A potential which is not single valued causes numerical difficulties when one attempts to find solutions for the wave functions needed to calculate overlap integrals. To avoid this problem the calculated potential for the B³ Σ state was used up to the vibrational level where the hook started to occur. First an extrapolation of the form a/r¹² was used. (This procedure is similar to that used by Halmann and Laulicht (Ref. 29) who used Vanderslice's potential for their calculations.) Using the resulting potential to find the maximum of the Shcumann-Runge continuum by the reflection method, one finds that it occurs at a much too high energy. An alternate method for constructing a more realistic potential in the troublesome region involves using the calculated potential at values of vibrational quantum number where one believes the calculation and using Evans and Schexander's (Ref. 30) values for the potential in the continuum portion of the potential and interpolating through the troublesome region. Franck-Condon factors were calculated using the so determined potentials.

*They claim no anomaly though.

Table 36*

POTENTIAL ENERGY FOR THE O₂ X³ Σ_g^- STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	789.81	1.15966	1.26310
1	2352.20	1.12759	1.30786
2	3891.68	1.10739	1.34156
3	5408.25	1.09177	1.37059
4	6901.91	1.07892	1.39709
5	8372.64	1.06791	1.42192
6	9820.43	1.05849	1.44586
7	11245.26	1.04980	1.46867
8	12647.12	1.04186	1.49078
9	14025.99	1.03482	1.51266
10	15381.88	1.02825	1.53410
11	16714.79	1.02215	1.55527
12	18024.69	1.01657	1.56737
13	19311.59	1.01136	1.59734
14	20575.48	1.00645	1.61823
15	21816.33	1.00183	1.63910
16	23034.10	0.99764	1.66018
17	21228.74	0.99367	1.68130
18	25400.22	0.98988	1.70249
19	26548.54	0.98618	1.72369
20	27673.62	0.98325	1.74566
21	28775.15	0.97498	1.76236
22	29852.56	0.97249	1.78501
23	30905.29	0.97124	1.80913

*From TURNGPT

Table 37*

POTENTIAL ENERGY FOR THE O₂ B³ Σ_u^- STATE

<u>v</u>	<u>v(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	353.45	1.52754	1.68252
1	1041.45	1.46883	1.75912
2	1706.55	1.45786	1.81448
3	2347.95	1.43628	1.86469
4	2965.55	1.41890	1.91241
5	3557.35	1.40495	1.96052
6	4118.45	1.39306	2.00873
7	4651.65	1.37998	2.05627
8	5153.05	1.36959	2.01829
9	5618.55	1.36125	2.16443
10	6047.45	1.35429	2.22607
11	6435.65	1.34833	2.29561
12	6781.05	1.34334	2.37479
13	7081.75	1.33902	2.46677
14	7336.75	1.33507	2.57613
15	7545.15	1.33088	2.70806
16	7714.11	1.32861	2.86245
17	7847.02	1.32627	3.04965
18	7949.15	1.32496	3.27710
19	8024.79	1.32740	3.56375
20	8077.44	1.33034	3.94952

*From TURNGPT

Table 38

MOLECULAR DATA NEEDED FOR TURNGPT ($O_2 X^3\Sigma_g^-$)

<u>v</u>	<u>Gv(cm⁻¹)</u>	<u>Bv(cm⁻¹)</u>
0	789.81	1.4375
1	2352.20	1.4215
2	3891.68	1.406
3	5408.25	1.3909
4	6901.91	1.3755
5	8372.64	1.3601
6	9820.43	1.343
7	11245.26	1.3296
8	12647.12	1.3145
9	14026.00	1.298
10	15381.88	1.2833
11	16714.79	1.2678
12	18024.69	1.2516
13	19311.59	1.236
14	20575.48	1.2204
15	21816.33	1.2046
16	23034.10	1.1870
17	24228.74	1.1711
18	25400.22	1.1550
19	26548.54	1.1390
20	27673.62	1.1226
21	28775.15	1.640
22	29852.56	1.0904
23	30905.29	1.0744

Table 39

MOLECULAR DATA NEEDED FOR TURNGPT (O_2 $B^3\Sigma_u^-$)

<u>v</u>	<u>Gv(cm⁻¹)</u>	<u>Bv(cm⁻¹)</u>
0	353.45	0.813
1	1041.45	0.798
2	1706.55	0.785
3	2347.95	0.770
4	2965.55	0.754
5	3557.35	0.735
6	4118.45	0.719
7	4652.65	0.703
8	5153.05	0.680
9	5618.55	0.655
10	6047.45	0.627
11	6435.65	0.596
12	6781.05	0.562
13	7081.75	0.525
14	7336.75	0.485
15	7545.15	0.443
16	7714.11	0.398
17	7847.02	0.354
18	7949.15	0.306
19	8024.79	0.258
20	8077.44	0.208
21	8109.38	0.159
22	8126.28	0.109

Table 39 (cont'd)

CONTINUUM VALUES

9150.0	1.31
9560.0	1.305
9970.0	1.300
10380.0	1.295
10780.0	1.290
11200.0	1.285
11640.0	1.28

Table 40

POTENTIAL ENERGY INPUT DATA USED FOR CALCULATING THE FRANCK-CONDON FACTORS FOR O₂ SCHUMANN-RUNGE BAND SYSTEMS

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	353.45	1.52754	1.68252
1	1041.45	1.46883	1.75912
2	1706.55	1.45786	1.81448
3	2347.95	1.43628	1.86469
4	2965.55	1.41890	1.91241
5	3557.35	1.40495	1.96052
6	4118.45	1.39306	2.00873
7	4652.65	1.37998	2.05627
8	5153.05	1.36959	2.10829
9	5618.55	1.36125	2.16443
10	6047.45	1.35429	2.22607
11	6435.65	1.34833	2.29561
12	6781.05	1.34334	2.37479
13	7081.75	1.33902	2.46677
14	7336.75	1.33507	2.57613

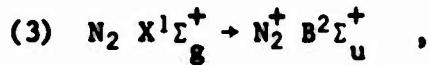
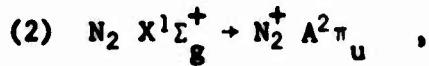
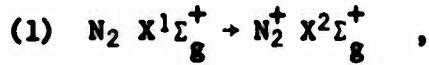
Table 40 (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
15	7545.15	---	2.70806
16	7714.11	---	2.86245
17	7847.02	---	3.04965
18	7949.15	---	3.27710
19	8024.79	---	3.56375
20	8077.44	---	3.94952

7. PHOTOIONIZATION FRANCK-CONDON FACTORS

a. N₂

The four photoionization transitions considered were



All five potentials used were generated using program TURNGPT and with the exception of the B state were generated from spectroscopic constants given by Gilmore (Ref. 21). The B state was generated by use of constants from Herzberg (Ref. 29).

Table 46 contains the spectroscopic data used. Tables 41 through 45 contain the generated potentials.

Table 41*

POTENTIAL ENERGY FOR THE $N_2 X^1\Sigma_g^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	1175.49	1.05485	1.14544
1	3505.14	1.02644	1.18417
2	5806.91	1.06820	1.21288
3	8078.91	0.99410	1.23755
4	10322.88	0.98242	1.25993
5	12538.14	0.97236	1.28081
6	14724.61	0.96349	1.30064
7	16882.22	0.95552	1.31968
8	19010.90	0.94829	1.33813
9	21110.57	0.94164	1.35612
10	23181.15	0.93550	1.37375
11	25222.58	0.92978	1.39111
12	27234.78	0.92443	1.40825
13	39317.67	0.91940	1.42522
14	31171.18	0.91464	1.44208
15	33095.24	0.91014	1.45884
16	34989.77	0.90586	1.47556
17	36854.69	0.90178	1.49224
18	38689.94	0.89788	1.50893
19	40495.43	0.89415	1.152564
20	52271.10	0.89056	1.54240

*From TURNGPT using Gilmore's constants.

Table 42*

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>
0	1099.54	1.07397	1.16768
1	3274.34	1.04461	1.20792
2	5416.60	1.02575	1.23791
3	7526.22	1.01120	1.26385
4	9603.09	0.99917	1.28752
5	11647.12	0.98884	1.30976
6	13658.25	0.97978	1.33100
7	15636.45	0.97170	1.35156
8	17581.70	0.96440	1.37161
9	19494.00	0.95777	1.39130
10	21373.38	0.95169	1.41075
11	23219.89	0.94611	1.43002
12	25033.61	0.94096	1.44919
13	26814.62	0.93619	1.46831
14	28563.05	0.93178	1.48743
15	30279.03	0.92768	1.50659
16	31962.72	0.92389	1.52582
17	33614.31	0.92037	1.54515
18	35233.99	0.91712	1.56462
19	36822.00	0.91412	1.58424
20	38378.58	0.91136	1.60404

*From TURNGPT using Gilmore's constants.

Table 43*

POTENTIAL ENERGY FOR THE $N_2^+ A^2\pi_u$ STATE				
<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	947.96	1.02656	1.22743	0.1175
1	2821.38	1.09570	1.27158	0.3498
2	4664.80	1.07615	1.30488	0.5783
3	6478.22	1.06118	1.33368	0.8031
4	8271.64	1.04887	1.38479	1.0242
5	10015.06	1.03838	1.38479	1.2416
6	11738.48	1.02917	1.40847	1.4553
7	13431.90	1.02097	1.43137	1.6652
8	15095.32	1.01357	1.45371	1.8714
9	16728.74	1.00681	1.47563	2.0739
10	18332.16	1.00061	1.49726	2.2727
11	19905.58	0.99487	1.51867	2.4678
12	21449.00	0.98954	1.53995	2.6791
13	22962.42	0.98455	1.56116	2.8468
14	24445.84	0.97987	1.58235	3.0307
15	25897.26	0.97546	1.60356	3.2109
16	27322.68	0.97130	1.62484	3.3880
17	28716.10	0.967356	1.64622	3.5601
18	30079.51	0.96361	1.66774	3.7291
19	31412.94	0.96003	1.68943	3.8944
20	32716.36	0.95662	1.71132	4.0560

*From TURNGPT using Gilmore's constants.

Table 44

POTENTIAL ENERGY FOR THE $N_2^+ B^2 \Sigma_u^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1197.15	1.03331	1.12304	0.1484
1	3588.66	1.00546	1.16196	0.4424
2	5887.46	0.98795	1.19199	0.7299
3	8147.86	0.97409	1.21811	1.0101
4	10344.26	0.96323	1.24330	1.2824
5	12467.06	0.95501	1.26903	1.5456
6	14508.06	0.94720	1.27401	1.7986
7	16469.16	0.94043	1.32000	2.0405
8	18291.36	0.93404	1.34765	2.2677
9	20018.26	0.92856	1.37643	2.4818
10	21614.96	0.92315	1.40798	2.6797
11	23094.86	0.91867	1.44118	2.8632
12	24466.26	0.91496	1.117632	3.0332
13	25742.56	0.91145	1.51208	3.1914
14	26938.86	0.90846	1.54832	3.3397
15	28065.46	0.90544	1.58452	3. 794
16	29132.56	0.90303	1.62095	3.6117
17	30148.06	0.90104	1.65763	3.7376
18	31114.06	0.89893	1.69439	3.8574
19	32036.06	0.89687	1.73160	3.9717
20	32858.06	0.89012	1.78474	4.0736

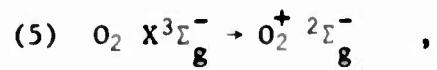
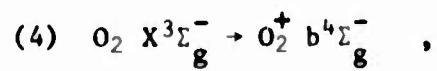
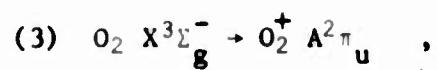
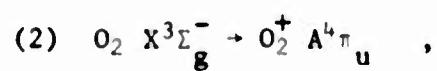
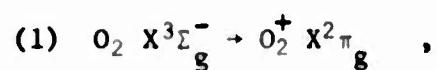
Table 45*

POTENTIAL ENERGY FOR THE $N_2^+ C^2\Sigma_u^+$ STATE				
<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1034.08	1.21465	1.31124	0.1282
1	3085.06	1.18158	1.34967	0.3824
2	5111.94	1.15962	1.37772	0.6337
3	7113.28	1.14238	1.49182	0.8818
4	9087.64	1.12798	1.42383	1.1266
5	11033.58	1.11558	1.44462	1.3679
6	12949.66	1.10471	1.46470	1.6054
7	14832.44	1.09508	1.48437	1.8091
8	16686.48	1.08646	1.50386	2.0687
9	18504.34	1.07874	1.52333	2.2941
10	20286.58	1.07182	1.54294	2.5150

*From TURNGPT using Gilmore's constants.

b. O₂

The photoionization transitions considered were



The seven potentials used were generated by program TURNGPT. The $O_2 X^3\Sigma_g^-$ state was generated by using data from Wallace (Ref. 24). This is the same potential that was used as the lower state of the O_2 S-R system. The six states of O_2^+ were all generated using the spectroscopic constants given by Gilmore (Ref. 21). These data are listed in table 53. The potentials are listed in tables 47 through 52.

Table 46

SPECTROSCOPIC CONSTANTS FOR N_2 PHOTOIONIZATION STATES

<u>We</u>	<u>W_{xe}</u>	<u>W_{ye}</u>	<u>W_{ze}</u>	<u>Be</u>	<u>ae</u>	<u>γe</u>	<u>re</u>
$N_2 X^1\Sigma_g^+$ state							
2358.07	14.188	-1.24 ⁻²	0.0	1.9987	0.0178	0.0	1.0976
$N_2 X^2\Sigma_g^+$ state							
2207.17	16.146	-2.85 ⁻²	9.2 ⁻⁴	1.9258	0.01743	-1.64 ⁻⁴	1.118
$N_2 A^2\Pi_u$ state							
1903.42	15.0	0.0	0.0	1.748	0.02	0.0	1.117
$N_2 B^2\Sigma_u^+$ state							
2418.7	22.53	-6.7 ⁻¹	4.0 ⁻²	2.083	0.0183	-1.65 ⁻³	1.075
$N_2 C^2\Sigma_u^+$ state							
2073.7	10.97	-2.4 ⁻¹	0.0	1.5124	0.0017	-7.5 ⁻⁴	1.262

Table 47*

POTENTIAL ENERGY FOR THE $O_2^+ X^2\Pi_g$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	934.12	1.07839	1.17354	0.1158
1	2777.56	1.04947	1.21552	0.3444
2	2587.94	1.03116	1.247.4	0.5678
3	6365.26	1.01714	1.26466	0.7891
4	8109.52	1.00561	1.29990	1.0054

Table 47* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
5	9820.72	0.99575	1.32370	1.2175
6	11498.86	0.98710	1.34652	1.4256
7	13143.94	0.97939	1.36865	1.6295
8	14755.96	0.97241	1.39030	1.8294
9	16334.92	0.96603	1.41161	2.0252
10	17880.82	0.96016	1.43268	2.2168
11	19393.66	0.95471	1.45362	2.4044
12	20873.44	0.94962	1.47448	2.5878
13	22320.16	0.94484	1.49534	2.7672
14	23733.82	0.94034	1.51624	2.9424

*From TURNGPT using Gilmore's constants.

Table 48*

POTENTIAL ENERGY FOR THE O ₂ ⁺ A ² _π _u STATE				
<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	446.08	1.34603	1.48386	0.0553
1	1317.68	1.30607	1.54794	0.1634
2	2161.88	1.28114	1.59762	0.2680
3	2978.68	1.26225	1.64192	0.3695
4	3768.08	1.24682	1.68348	0.4672
5	4530.08	1.23364	1.72353	0.5616
6	5246.68	1.22209	1.76277	0.6505
7	5971.88	1.21173	1.80167	0.7404
8	6651.88	1.20230	1.84057	0.8246
9	7304.08	1.19358	1.87975	0.9055
10	7929.08	1.08541	1.91945	0.9830

*From TURNCPPT using Gilmore's constants.

Table 49*

POTENTIAL ENERGY FOR THE $O_2^+ b^4\pi$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	594.11	1.22498	1.34439	0.0736
1	1756.70	1.19030	1.39967	0.2178
2	2885.11	1.16869	1.44240	0.3577
3	3979.34	1.15234	1.48038	0.4933
4	509.39	1.13900	1.51592	0.6248
5	6065.26	1.12765	1.55006	0.7520
6	7056.95	1.11772	1.58341	0.8749
7	8014.46	1.10886	1.61637	0.9936
8	8937.79	1.10082	1.64922	1.1081
9	9826.94	1.09343	1.68218	1.2183
10	10681.91	1.08656	1.71545	1.3243

*From TURNGPT using Gilmore's constants.

Table 50*

POTENTIAL ENERGY FOR THE $O_2^+ a^4\pi$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	515.25	1.32207	1.45020	0.0639
1	1530.05	1.28390	1.50774	0.1897
2	2425.29	1.25993	1.55142	0.3130
3	3497.64	1.24174	1.58969	0.4336
4	4450.21	1.22690	1.62500	0.5517
5	5382.00	1.21429	1.65846	0.6672
6	6293.01	1.20332	1.69071	0.7802
7	7183.24	1.19358	1.72214	0.8906

Table 50* (cont'd)

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
8	8052.60	1.18484	1.75304	0.9983
9	8901.36	1.17690	1.78360	1.1036
10	9729.25	1.16963	1.81397	1.2062

*From TURNGPT using Gilmore's constants.

Table 51*

POTENTIAL ENERGY FOR THE O₂⁺ c^{4Σ_u⁻ STATE}

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	1195.50	1.14677	1.23086	0.1482
1	3559.50	1.12238	1.26895	0.4413
2	5887.50	1.10740	1.29783	0.7299
3	8079.50	1.09628	1.32307	1.0141
4	10435.50	1.08740	1.34627	1.2938
5	12655.50	1.08006	1.368916	1.8390
6	14839.50	1.07383	1.28917	1.8398
7	16987.50	1.06847	1.40954	2.1060
8	19099.50	1.06382	1.42945	2.3679
9	21175.50	1.05974	1.44904	2.6253
10	23215.50	1.05916	1.46839	2.8782

*From TURNGPT using Gilmore's constants.

Table 52*

POTENTIAL ENERGY FOR THE $O_2^+ 2\Sigma_g^-$ STATE				
<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	360.50	1.28272	1.43501	0.0447
1	1066.50	1.23627	1.50491	0.1322
2	1752.50	1.20657	1.55759	0.2173
3	2418.50	1.18361	1.60411	0.2998
4	3064.50	1.16440	1.64740	0.3799
5	3690.50	1.14791	1.68880	0.4575
6	4296.50	1.13310	1.72910	0.5327
7	4882.50	1.11970	1.76878	0.6053
8	5448.50	1.10730	1.80821	0.6755
9	5994.50	1.09572	1.84768	0.7432
10	6520.50	1.08478	1.88740	0.8084

*From TURNGPT using Gilmore's constants.

Table 53

SPECTROSCOPIC CONSTANTS FOR O₂ PHOTOIONIZATION STATES

<u>We</u>	<u>W_{xe}</u>	<u>W_{ye}</u>	<u>W_{ze}</u>	<u>B_e</u>	<u>ae</u>	<u>γe</u>	<u>re</u>
$O_2^+ X^2\Sigma_g$ state							
1876.50	16.53	0	0	1.67220	0.01984	0.0	1.12270
$O_2^+ a^4\Sigma_u$ state							
1035.69	10.39	0	0	1.10461	0.01575	0.0	1.38126
$O_2^+ A^2\Sigma_u$ state							
899.00	13.70	0	0	1.06170	0.01906	-1.95 ⁻⁴	1.40890
$O_2^+ b^4\Sigma_g^-$ state							
1196.77	17.09	0	0	1.28729	0.02206	0.0	1.27953

Table 53 (cont'd)

<u>We</u>	<u>Wexe</u>	<u>Weye</u>	<u>Weze</u>	<u>Be</u>	<u>ae</u>	<u>ye</u>	<u>re</u>
<u>O₂⁺ 2Σ⁻ state</u>							
726.00	10.00	0	0	1.15000	0.01700	0.0	estimated
<u>O₂⁺ c^{4Σ⁻}</u> state							
2400.00	18.00	0	0	1.50000	0.02000	0.0	estimated

SECTION III

TABLES OF FRANCK-CONDON FACTORS

This section contains tables of the Franck-Condon factors calculated from the data given in Section II. In Appendix I is a listing of program TURNGPT which was used to generate the input data for program FRANKON. The Franck-Condon factors have been calculated by program FRANKON which is listed in Appendix II.

Table 94 contains a list of R-K-R Franck-Condon factor tabulations known to the authors at the time this work was started. This list includes only transitions of interest for atmospheric diatomic molecules.

Table 54

222 FRANC-CONJON FACTORS FOR CN RED (11/21)

	V	J	1	2	3	4	5	6	7	8	9	
1	4.991-	1	3.719-	1	1.146-	1	1.702-	2	1.409-	3	1.774-	3
2	3.190-	1	4.573-	2	3.532-	1	2.222-	1	5.312-	2	5.259-	3
3	1.254-	1	2.397-	1	1.248-	2	2.145-	1	2.884-	1	1.030-	1
4	3.922-	2	1.333-	1	9.735-	<	9.064-	2	9.621-	2	2.995-	1
5	1.159-	2	9.034-	2	1.793-	1	1.467-	2	1.544-	1	1.034-	2
6	3.127-	3	3.532-	2	1.335L-	1	1.197-	1	2.353-	3	1.533-	1
7	6.302-	4	1.229-	2	6.943-	2	1.336-	1	5.541-	2	3.277-	2
8	2.144-	4	4.350-	3	2.949-	2	9.517-	2	1.173-	1	1.272-	2
9	5.060-	5	1.249-	3	1.160-	<	0.377-	2	1.034-	1	7.352-	2
10	1.469-	5	3.734-	4	3.347-	3	2.234-	2	5.903-	2	7.756-	2
11	3.807-	6	1.164-	4	1.355-	3	9.142-	3	1.345-	1	1.034-	1
12	1.052-	6	3.232-	5	4.541-	4	3.533-	3	1.722-	2	1.187-	2
13	3.064-	7	9.733-	6	1.476-	4	1.315-	3	7.629-	3	2.759-	2
14	9.037-	6	2.377-	6	4.638-	>	4.775-	4	3.072-	3	1.342-	2
15	2.816-	3	9.462-	7	1.298-	>	1.709-	4	1.227-	3	1.101-	3
16	8.738-	9	3.053-	7	2.353-	<	0.031-	5	0.711-	4	2.031-	3
17	2.575-	9	1.037-	7	1.022-	6	2.156-	5	1.844-	4	1.117-	3
18	6.820-10	3	3.258-	3	6.226-	7	7.717-	6	5.933-	5	4.503-	4
19	1.519-11	9	9.979-	9	2.088-	7	2.764-	5	2.595-	5	1.932-	4

Table 54 (cont'd)
(2N RE) (1/2)

v	w	x	y	z	11	12	13	14	15	16	17	18
1	2.0760-11	3.0355-11	2.0139-12	0.749-12	3.332-12	3.983-12	2.534-12	6.128-12	1.039-14			
1	2.0497-3	1.3597-11	5.05/3-10	1.0302-10	7.015-10	6.357-11	6.393-12	3.451-11	4.029-13			
2	8.046-	9.1259-	9.0143-10	6.000-11	6.037-11	5.033-11	2.084-10	2.307-10	3.147-11			
3	3.560-	5.0332-	9.2.137-	9.1.291-10	1.195-11	2.125-11	1.426-11	7.944-12	1.626-11			
4	3.436-	4.0.062-	3.7.046-	3.2.916-9	1.531-9	9.333-10	7.336-10	1.661-11	4.463-12			
5	1.133-	2.7.0243-	4.2.040-	5.2.047-	7.2.028-11	2.0.523-	9.3.919-9	1.0.811-9				
5	1.136-	1.1.066-	2.1.0307-	3.0.0462-	5.0.049-	7.0.642-12	7.2.48-13	9.501-12	2.432-13			
7	2.720-	1.1.073-	1.2.060-	2.0.014-	3.0.621-	5.0.392-	7.0.547-10	6.0.663-12	5.0.633-9			
9	2.757-	2.2.074-	1.1.0.5-	1.0.159-	2.0.965-	3.0.332-	4.0.966-	1.0.495-	0.4266-	3		
9	1.271-	1.4.069-	3.2.035-	1.2.014-	1.5.731-	2.6.154-	3.2.722-	4.0.263-	6.0.543-	3		
10	5.410-	4.1.331-	1.1.010-	3.1.097-	1.2.0.370-	1.7.0.500-	2.9.237-	3.4.590-	4.7.346-	0		
11	6.342-	2.1.297-	2.1.0155-	1.1.0454-	2.1.0457-	1.2.0.546-	1.9.728-	2.1.342-	2.7.159-	4		
12	7.529-	2.3.058-	2.3.0527-	2.0.950-	2.3.0.826-	2.1.0.019-	2.0.629-	1.1.207-	1.1.665-	2		
13	1.031-	2.7.0751-	2.1.0208-	2.5.903-	2.5.911-	2.6.0.577-	2.6.291-	2.2.600-	1.1.453-	1		
14	1.0214-	3.3.050-	2.6.075-	2.9.790-	4.7.734-	2.3.116-	2.9.0.76-	2.3.226-	2.6.24-	4		
15	2.628-	2.1.321-	3.5.0205-	2.4.943-	2.1.953-	3.8.0.593-	2.1.0.379-	2.1.0.379-	1.1.223-	2		
15	5.020-	2.1.037-	2.1.0.07-	2.6.0.34-	2.2.0.932-	2.1.0.263-	2.0.332-	2.0.332-	2.0.633-	4		
17	5.926-	2.3.015-	2.1.0467-	3.2.347-	2.5.969-	2.1.227-	2.0.637-	2.0.637-	2.1.146-	1		
19	5.144-	2.5.163-	2.2.033-	2.5.630-	4.3.631-	2.5.0.911-	2.2.0.070-	3.4.456-	2.5.381-	2		

Table 55

KK2 FRANCK-CONDON FACTORS FOR CN RED (3/2)

V	VV	J	1	2	3	4	5	6	7	8	9	
1	4.922-	1	3.715-	1	1.125-	1	1.911-	2	1.607-	3	1.739-	3
2	3.267-	1	4.327-	2	3.483-	1	2.239-	1	3.353-	2	2.272-	3
3	1.226-	1	2.431-	1	1.152-	2	2.139-	1	2.632-	1	1.025-	5
4	3.868-	2	1.358-	1	1.052-	1	1.705-	2	9.437-	2	1.074-	4
5	1.493-	2	9.453-	2	1.844-	1	1.606-	2	1.475-	1	1.025-	3
6	2.945-	3	3.527-	2	1.346-	1	1.259-	1	1.333-	3	1.593-	4
7	7.384-	4	4.154-	2	6.666-	2	1.432-	1	2.013-	2	1.298-	1
8	1.349-	4	3.599-	3	2.701-	2	9.436-	2	1.242-	1	1.725-	2
9	4.556-	2	1.332-	3	9.776-	3	4.707-	2	1.039-	1	9.835-	2
10	9.557-	6	2.356-	4	3.368-	3	1.994-	2	5.756-	2	1.039-	1
11	1.772-	6	7.531-	5	1.065-	3	7.659-	3	3.324-	2	9.292-	2
12	3.256-	7	1.825-	5	3.226-	4	2.777-	3	1.467-	2	4.052-	2
13	7.821-	6	6.210-	6	9.081-	5	9.568-	4	5.933-	3	9.317-	2
14	3.229-	6	2.133-	6	2.396-	5	3.089-	4	2.243-	3	1.281-	2
15	1.696-	6	3.034-	7	6.221-	6	9.269-	5	8.062-	4	9.09-	3
16	3.723-	9	4.412-	6	5.286-	7	7.054-	6	5.536-	5	3.568-	4
17	4.587-10		2.532-	8	1.746-	7	1.985-	6	2.458-	5	2.279-	4
18	6.999-11		3.534-	9	4.907-	8	5.916-	7	6.711-	6	5.219-	5

Table 55 (cont'd)
(CV REC (3/2))

	V	VV	16	11	12	13	14	15	16	17	18	
0	9.057-10	3.486-	9	3.915-13	1.085-	9	1.209-13	8.045-13	2.631-11	3.035-13	2.032-10	
1	1.145-7	1.0753-	3	1.346-	7.645-	9	9.637-13	2.013-	1.176-11	1.0428-	1.0533-11	
2	7.130-	9	8.642-	3	5.935-	8	2.411-	9	3.152-	9	1.050-10	
3	4.592-	6	2.183-	9	8.071-	8	6.016-	8	2.534-	8	1.024-9	
4	2.869-	4	9.517-	6	2.012-	8	6.479-	8	6.331-	9	2.070-9	
5	1.617-	2	5.924-	4	1.072-	5	7.025-	6	7.198-	8	1.027-8	
6	1.082-	1	2.663-	2	1.203-	3	3.692-	5	2.373-	7	3.051-	8
7	2.736-	1	1.498-	1	2.531-	2	1.925-	3	6.545-	5	3.928-	7
8	3.614-	2	2.637-	1	1.713-	1	3.648-	2	3.119-	3	1.115-	4
9	1.212-	1	6.748-	3	2.444-	1	2.022-	1	5.008-	2	4.791-	3
10	3.442-	5	1.292-	1	6.513-	7	2.072-	1	2.285-	1	6.611-	2
11	7.171-	2	6.699-	3	1.219-	1	7.047-	3	1.679-	1	2.492-	1
12	6.863-	2	4.674-	2	2.425-	2	1.005-	1	2.513-	2	1.268-	1
13	1.026-	2	7.596-	2	2.095-	2	4.650-	2	7.397-	2	4.915-	2
14	5.871-	3	2.578-	2	7.149-	2	5.291-	3	6.627-	2	6.553-	2
15	3.956-	2	7.0475-	3	4.162-	2	5.892-	2	2.368-	5	7.952-	2
16	6.396-	2	2.152-	2	3.071-	3	5.372-	2	6.150-	2	6.256-	3
17	6.441-	2	3.050-	2	8.003-	3	1.261-	2	2.680-	2	2.380-	2
18	5.029-	2	3.123-	2	3.492-	2	9.372-	4	2.471-	2	3.535-	2

Table 56

RRR FRANC<-NCNC>-C11-C12-C13-C14

VV	0	1	2	3	4	5	6	7	8	9
V	9.262-1	7.361-2	5.536-3	3.828-4	2.634-5	1.416-6	2.520-7	7.579-8	1.178-11	3.403-9
U	7.956-2	7.911-1	1.246-1	1.434-2	1.237-3	9.332-4	3.435-5	2.544-6	4.200-7	3.962-14
1	2.172-3	1.424-1	6.723-1	1.543-2	2.393-3	2.670-4	2.327-5	1.554-6	1.019-7	6.002-7
2	3.1263-0	2.651-3	1.904-1	5.941-1	1.739-1	3.332-2	4.555-3	5.417-4	5.309-5	7.050-6
3	4.6316-7	2.597-3	4.113-3	2.313-1	5.231-1	1.023-1	4.92-2	7.036-3	1.049-3	1.402-4
4	3.10325-7	1.719-6	7.727-7	5.304-3	2.662-4	4.832-5	1.779-6	5.526-7	3.804-8	1.710-3
5	0.1244-7	1.233-7	3.906-0	2.430-4	6.976-2	2.326-1	4.399-1	1.638-1	6.403-2	1.236-2
6	7.61243-9	9.949-9	6.326-8	1.671-7	3.933-4	3.156-3	3.596-1	4.539-1	1.422-1	7.061-2
7	6.679-6	2.507-3	2.614-7	5.739-7	4.179-5	1.619-3	6.317-4	3.122-1	4.756-1	1.146-1
8	9.1356-8	2.763-6	4.349-5	3.052-7	3.456-6	6.435-5	3.151-3	1.556-6	2.953-1	5.190-1
9	10.5341-9	1.360-7	1.227-9	4.041-7	7.297-9	1.523-5	1.025-5	5.010-3	5.041-3	2.532-1
10	11.1047-8	2.359-8	2.399-9	2.390-8	4.639-7	1.971-6	4.111-5	2.174-5	6.664-3	2.046-2
11	12.6857-10	6.952-9	3.511-3	3.943-9	1.315-7	2.514-3	3.592-7	6.627-5	3.395-4	6.386-3
12	13.1522-9	2.354-8	7.378-10	1.102-10	2.673-8	1.166-7	1.957-7	3.555-6	7.617-5	1.434-3
13	14.1.915-9	1.239-8	2.556-8	3.205-11	1.040-7	3.979-3	2.924-9	4.146-7	1.632-5	2.239-5
14	15.6.215-11	3.152-10	5.003-8	1.452-8	4.653-8	2.293-7	1.335-7	3.070-7	5.303-7	5.109-5
15	16.6.715-10	1.364-9	2.629-8	5.354-8	1.916-8	2.315-7	1.697-7	1.642-7	1.247-6	6.005-7
16	17.1.443-9	1.315-9	2.863-9	5.754-8	3.020-8	1.142-7	2.911-7	2.036-7	2.609-7	2.403-6
17	18.7.204-10	4.356-11	9.781-11	2.303-8	4.994-8	1.037-8	3.059-7	2.341-7	1.467-7	1.297-6

Table 56 (cont'd)
(3N VIJ-EII)

y	VV	10	11	12	13	14	15	16	17	18
3	2.075-	9	5.363-	9	2.151-13	6.289-11	1.038-10	3.534-11	9.761-10	1.965-9
4	7.051-	8	1.055-	7	9.603-	8	6.497-	9	7.634-	9
2	2.453-	7	1.037-	7	2.225-	7	1.550-	7	2.154-	8
3	2.651-	5	1.336-	5	5.076-	7	1.849-	7	5.918-	8
4	2.044-	5	2.099-	5	2.627-	6	7.979-	7	3.531-	9
5	2.763-	6	4.448-	5	9.053-	6	3.029-	6	6.069-	7
3	2.436-	3	4.0265-	4	7.0419-	5	2.184-	5	2.227-	5
7	1.447-	2	3.032-	3	5.511-	4	9.034-	5	1.561-	5
8	7.637-	2	1.0443-	2	3.716-	3	6.590-	4	1.138-	4
3	6.146-	2	6.234-	2	1.342-	2	4.122-	3	7.116-	4
10	5.011-	1	4.915-	2	9.001-	2	1.107-	2	4.537-	3
11	1.090-	1	6.056-	1	2.231-	2	1.022-	1	7.776-	3
12	4.0820-	2	1.0126-	1	6.974-	1	4.774-	3	1.194-	1
13	3.656-	3	9.557-	2	4.234-	2	7.135-	1	6.163-	3
14	3.358-	3	3.491-	4	1.202-	1	2.452-	3	6.766-	1
15	3.050-	5	5.0468-	3	2.219-	3	1.375-	1	1.626-	2
16	7.461-	5	5.115-	4	5.015-	3	1.613-	2	1.229-	1
17	1.244-	3	4.596-	3	1.993-	3	2.921-	3	4.671-	2
18	6.677-	7	3.041-	5	6.002-	6	3.995-	3	5.681-	5

TABLE 57
FRANCK-CCONDON FACTORS FOR LIQUIDS

	1	2	3	4	5	6	7	8	9	10	11	12
V	2.000-1	2.905-1	1.396-1	3.705-2	3.415-2	9.172-3	2.037-3	3.939-4	5.474-5	7.798-6	9.967-7	2.204-3
1	2.188-1	1.253-1	2.352-3	7.793-2	1.973-1	1.659-1	1.040-1	4.355-2	2.16-2	5.395-4	5.395-4	1.231-5
2	2.370-1	1.134-2	9.147-2	1.0123-1	3.356-3	6.352-2	1.717-1	1.561-1	9.233-2	3.652-3	2.562-3	5.162-4
3	1.943-1	2.357-2	1.150-1	1.013-4	9.433-2	7.746-2	1.763-2	7.351-2	1.653-1	1.653-1	2.319-2	9.673-3
4	1.176-1	9.359-2	3.029-2	6.216-2	6.057-2	1.051-2	1.021-1	4.254-2	6.954-3	1.330-1	1.385-1	1.210-1
5	6.620-2	1.243-1	1.243-3	9.026-4	8.526-2	1.579-2	4.135-2	9.345-2	1.348-2	2.776-2	1.216-1	1.470-1
6	3.443-2	1.182-1	3.034-2	3.354-2	4.967-2	3.460-2	3.013-2	6.763-2	1.215-4	7.460-2	6.460-2	2.050-4
7	1.667-2	9.723-2	9.275-2	5.730-4	7.353-2	1.422-3	6.964-2	3.213-4	6.575-2	2.717-2	1.954-2	2.964-2
8	7.165-3	2.572-2	9.756-2	1.0319-2	3.722-2	6.174-2	2.074-2	4.077-2	3.246-2	1.961-2	6.633-2	1.299-3
9	3.552-3	3.190-2	6.555-2	3.144-2	3.219-3	5.147-2	2.106-3	5.363-2	2.334-3	3.999-2	9.029-4	5.525-2
10	1.531-3	1.739-2	6.920-2	7.456-2	5.069-3	3.613-2	3.392-2	1.425-2	4.248-2	1.349-2	3.747-2	3.130-2
11	6.263-4	5.993-3	4.319-2	7.783-2	3.146-2	6.414-3	5.293-2	1.781-3	4.537-2	3.366-3	4.529-2	3.164-3
12	2.716-4	4.471-3	2.656-2	6.653-2	5.526-2	1.393-3	3.511-2	2.561-2	1.136-2	4.805-2	4.765-3	4.212-2
13	1.167-4	2.168-3	1.557-2	4.384-2	6.602-2	1.681-2	9.674-3	4.363-2	1.814-3	3.635-2	9.659-3	3.313-2
14	4.314-5	1.029-3	9.392-3	3.334-2	6.268-2	3.957-2	1.957-2	3.428-2	1.958-2	1.867-2	3.652-2	2.015-3
15	1.035-5	4.706-4	4.549-3	2.155-2	5.183-2	5.375-2	8.912-3	1.363-2	3.573-2	2.648-4	3.397-2	2.541-2
16	6.082-6	2.403-4	2.310-3	1.296-2	3.050-2	5.676-2	2.613-2	6.379-4	3.229-2	1.296-2	1.149-2	3.399-3
17	2.272-6	8.914-5	1.146-3	7.476-3	2.678-2	5.167-2	4.119-2	2.871-3	1.690-2	2.752-2	3.794-5	5.118-2
18	3.597-7	3.615-5	5.470-4	4.154-3	1.758-2	4.197-2	4.669-2	4.958-2	3.561-3	2.912-2	6.686-3	1.395-2
19	3.251-7	1.366-5	2.693-4	2.234-3	1.098-2	3.146-2	4.821-2	2.783-2	4.556-4	1.927-2	1.854-2	2.019-2
20	1.152-7	4.333-6	1.356-4	1.125-3	6.416-3	2.155-2	4.110-2	3.556-2	5.293-3	7.398-3	2.270-2	1.569-3
												1.602-2

Table 57 (cont'd)

(CO 474. 0)

y	VV	13	14	15	16	17	18	19	20	21	22	<3	24	
5	6.861-	6	2.942-	3	1.339-	6	2.653-10	1.6425-	9	1.033-	9	1.175-10	5.411-11	
4	2.896-	5	3.797-	7	3.562-	9	2.652-	6	2.536-	3	1.130-	8	3.691-	9
2	3.685-	5	1.514-	5	1.932-	6	8.523-14	1.287-	8	3.429-	8	5.712-	5	
3	2.162-	3	6.266-	4	6.231-	5	3.944-	6	2.258-	7	3.884-	7	1.846-	7
4	2.298-	2	6.476-	3	1.372-	3	2.250-	4	3.812-	5	5.531-	6	2.887-	6
5	1.006-	1	4.633-	2	1.355-	2	3.954-	3	6.382-	4	1.355-	4	2.723-	3
6	2.362-	1	1.322-	1	7.946-	2	3.265-	2	1.431-	2	2.826-	3	5.467-	4
7	7.496-	3	6.896-	2	1.642-	1	1.121-	1	5.895-	2	2.876-	2	5.377-	3
8	7.177-	2	5.233-	3	3.216-	2	1.141-	1	1.353-	1	1.422-	2	6.238-	2
9	9.980-	3	7.644-	2	4.147-	2	9.498-	4	5.489-	2	1.332-	1	1.205-	1
10	6.209-	2	4.521-	3	3.644-	2	7.322-	2	1.352-	2	1.635-	2	9.599-	2
11	1.910-	3	4.538-	2	3.781-	2	3.193-	3	6.457-	2	5.856-	2	2.585-	4
12	3.303-	2	3.442-	2	3.114-	3	5.814-	2	6.911-	3	2.377-	2	7.145-	2
13	3.939-	2	2.961-	3	3.036-	2	3.246-	3	3.710-	2	6.150-	2	6.118-	4
14	1.925-	3	3.985-	2	8.245-	3	2.995-	2	3.114-	2	5.038-	3	5.487-	2
15	1.468-	2	2.562-	2	1.193-	2	3.576-	2	2.144-	3	1.298-	2	3.663-	3
16	3.547-	2	1.644-	2	3.737-	2	1.085-	3	3.676-	2	6.998-	3	2.6426-	2
17	2.138-	2	1.451-	2	1.765-	2	1.632-	2	2.266-	2	9.338-	3	5.376-	2
18	1.692-	3	3.033-	2	1.914-	5	3.228-	2	1.412-	5	3.371-	2	1.454-	3
19	3.751-	3	2.012-	2	1.226-	2	1.430-	2	1.513-	2	1.381-	2	2.498-	2
20	1.616-	2	3.641-	3	2.352-	2	3.470-	4	2.586-	2	2.239-	5	2.731-	2

Table 58 RRR FRANCK-COURAN FACTORS $\Sigma \Sigma$ ($\pi(2)$ 151.0)

V	W	J	1	2	3	4	5	6
3	4.033-	1	3.394-	1	1.662-	1	6.68J-	2
4	3.990-	1	2.963-	3	1.589-	1	1.963-	1
2	1.616-	1	2.74J-	1	6.860-	2	2.203-	2
3	3.411-	2	2.767-	1	9.595-	2	1.245-	1
4	4.01J-	3	9.592-	2	2.973-	1	1.515-	1
5	2.655-	4	1.628-	2	1.680-	1	2.431-	1
6	1.066-	2	1.424-	3	3.093-	2	2.295-	1
7	2.527-	7	6.538-	5	4.337-	3	7.163-	2
8	3.912-	9	1.398-	6	2.337-	4	9.082-	3
9	2.559-1J	3	5.579-1J	11	5.539-	6	6.333-	7
10	3.15J-	9	1.243-12	12	1.357-	4	1.660-	5
11	3.23J-1J	2	1.93-	9	3.377-12	6	925-	5
12	4.427-1J	10	1.135-	3	2.924-	3	9.562-1J	12
13	5.016-1J	7	5.332-11	11	6.955-1J	20	82J-	9
14	4.666-12	8	4.91-10	10	1.1A1-1J	11	1.285-	9
15	1.209-14	3	3.364-10	10	6.717-1J	4	3.077-1J	13
16	7.521-11	1	826-11	5	9.34-1J	10	40J-	9
17	1.011-14	2	320-10	4	560-11	3	595-1J	11

Table 58 (cont'd)

	VV	7	8	9	10	11	12	13
Y	8.221-	4	2.611-	4	8.295-	5	2.645-	5
1	1.127-	2	4.262-	3	1.572-	3	5.745-	4
2	5.617-	2	2.722-	2	1.214-	2	5.153-	3
3	1.114-	1	6.886-	2	4.727-	2	2.482-	2
4	5.489-	2	9.391-	2	8.975-	2	6.509-	2
5	9.739-	3	1.444-	2	5.953-	2	6.133-	2
6	1.843-	1	3.335-	2	5.372-	1	2.511-	2
7	3.054-	3	8.142-	2	6.755-	2	4.064-	2
8	1.280-	1	4.732-	3	4.454-	2	7.713-	2
9	1.309-	4	1.199-	1	2.917-	2	1.356-	2
10	2.854-	1	1.822-	2	8.952-	2	5.092-	2
11	2.334-	1	1.514-	1	3.875-	2	5.163-	2
12	7.292-	2	2.591-	1	9.664-	2	7.261-	2
13	6.519-	3	9.348-	2	2.722-	1	5.003-	2
14	3.665-	4	1.341-	2	1.296-	1	2.712-	1
15	3.597-	6	6.387-	4	2.008-	2	1.611-	1
15	3.126-	9	6.543-	5	1.858-	3	2.871-	2
17	1.417-	9	3.135-12	1	0.855-	5	1.622-	3
							3.950-	2

Table 59

TABLE FRACTION-CONCENTRATION FACTORS FOR (V12) 27.0

	VV	0	1	2	3	4	5	6	7	8
0	4.524-	1	3.272-	1	1.459-	1	5.162-	2	1.656-	2
1	3.925-	1	2.177-	2	2.036-	1	1.993-	1	1.114-	1
2	1.331-	1	3.415-	1	2.420-	2	6.317-	2	1.644-	1
3	2.043-	2	2.930-	1	2.102-	1	8.923-	2	4.746-	3
4	9.693-	4	5.364-	2	3.307-	1	1.199-	1	1.131-	1
							3.915-	3	4.031-	2
							4.031-	1	1.001-	1

	VV	9	10	11	12	13	14	15	16	17
0	2.180-	5	2.433-	5	1.354-	5	3.454-	7	3.229-	9
1	5.436-	4	1.594-	4	4.212-	5	1.268-	5	3.563-	6
2	5.320-	3	1.036-	3	6.070-	4	1.951-	4	9.139-	5
3	2.620-	2	2.111-	2	4.344-	3	1.606-	3	2.719-	4
4	6.802-	2	3.736-	2	1.736-	2	7.870-	3	3.217-	3
							1.246-	3	4.650-	4
							1.667-	4	1.667-	5

Table 60

2X2 FRANCK-CONDON FACTORS F2(F2 0-M 1)

ν'	0	1	2	3	4	5	6	7	8	9	10	
1	2.753-	7	3.797-	6	2.719-	5	5.022-	4	1.540-	3	3.989-	3
1	3.751-	6	4.532-	5	2.822-	4	2.822-	4	3.819-	3	9.818-	2
2	2.592-	5	2.723-	4	1.461-	3	1.461-	3	2.939-	2	6.346-	2
3	1.212-	4	1.497-	3	2.032-	3	3.263-	2	5.400-	2	6.741-	2
4	6.314-	4	3.331-	3	1.277-	2	1.277-	2	6.533-	2	3.330-	2
5	1.247-	3	6.106-	3	2.562-	2	2.562-	2	6.393-	2	5.074-	2
6	3.449-	3	1.645-	2	4.165-	2	4.165-	2	5.373-	2	2.066-	2
7	6.493-	3	2.855-	2	3.874-	2	5.674-	2	2.847-	2	9.719-	2
8	1.228-	2	4.306-	2	6.390-	2	6.390-	2	5.638-	3	6.534-	3
9	2.098-	2	5.668-	2	5.989-	2	5.989-	4	2.591-	2	3.292-	2
10	3.279-	2	6.606-	2	4.312-	2	4.312-	2	1.402-	2	3.553-	2
11	4.729-	2	6.725-	2	2.222-	2	2.222-	2	3.853-	2	2.524-	2
12	6.331-	2	5.899-	2	5.482-	3	5.482-	3	3.456-	2	7.160-	3
13	7.908-	2	4.273-	2	5.620-	5	5.620-	5	2.310-	3	6.712-	3
14	9.239-	2	2.355-	2	7.135-	3	7.135-	3	7.863-	3	9.048-	3
15	1.017-	1	7.493-	3	2.158-	2	2.158-	2	5.962-	8	2.231-	2
16	1.047-	1	1.142-	4	3.454-	2	3.454-	2	6.511-	3	2.537-	2
17	1.003-	1	4.477-	3	3.021-	2	3.021-	2	1.907-	2	1.550-	2
18	6.919-	2	1.915-	2	3.054-	2	3.054-	2	2.567-	2	3.350-	3
19	7.193-	2	3.759-	2	1.646-	2	1.646-	2	2.055-	2	3.512-	2
20	1.534-	2	1.766-	2	7.272-	4	7.272-	4	2.100-	3	2.975-	3

Table 60 (cont'd)

RKFRANC(=JONJON FACTORS = J2(42 3-H 21)

	W	11	12	13	14	15	16	17	18	19	20	21						
V	6.934-	2	9.611-	2	1.068-	1	1.162-	1	1.064-	1	0.976-	2	0.972-	2	0.972-	2		
1	7.515-	2	5.404-	2	2.085-	2	5.341-	3	5.599-	4	1.446-	2	1.135-	2	0.914-	2	0.493-	2
2	7.815-	3	3.945-	4	1.530-	2	4.360-	2	5.696-	2	0.62-	2	2.720-	2	4.977-	3	1.586-	3
3	1.663-	2	4.061-	2	4.726-	2	2.343-	2	5.803-	3	1.737-	3	2.223-	2	4.635-	2	4.971-	2
4	4.334-	2	2.002-	2	4.550-	3	3.159-	3	2.538-	2	4.208-	2	3.030-	2	6.737-	3	1.812-	3
5	1.246-	2	1.711-	4	1.712-	2	3.052-	2	2.001-	2	4.025-	3	3.566-	3	2.697-	2	3.929-	2
6	3.652-	3	2.620-	2	3.264-	2	1.158-	2	4.190-	4	1.914-	2	3.453-	2	1.913-	2	3.786-	4
7	2.903-	2	2.600-	2	3.552-	3	5.739-	3	2.779-	2	2.565-	2	3.600-	3	5.771-	3	2.966-	2
8	2.163-	2	1.024-	3	1.056-	2	2.669-	2	1.593-	2	2.013-10	10	1.623-	2	2.934-	2	1.996-	2
9	2.916-	4	1.233-	2	2.764-	2	1.331-	2	1.231-	3	2.143-	2	2.326-	2	2.398-	3	0.264-	3
10	1.119-	2	2.619-	2	0.346-	3	2.449-	3	2.273-	2	1.797-	2	1.374-	4	1.448-	2	2.112-	2
11	2.520-	2	9.665-	3	2.237-	3	2.244-	2	1.522-	2	3.521-	3	1.536-	2	2.091-	2	1.326-	3
12	1.240-	2	9.616-	4	1.996-	2	1.513-	2	4.337-	5	1.679-	2	1.821-	2	3.137-	4	1.350-	2
13	2.205-	7	1.630-	2	1.699-	2	5.047-	5	1.474-	2	1.748-	2	2.356-	4	1.354-	2	1.057-	2
14	1.057-	2	1.937-	2	1.143-	3	1.141-	2	1.821-	2	7.130-	4	1.175-	2	1.732-	2	4.054-	4
15	2.035-	2	4.592-	3	3.129-	3	1.392-	2	2.413-	3	0.475-	3	1.791-	2	9.931-	4	1.098-	2
16	1.090-	2	1.459-	3	1.612-	2	6.347-	3	4.310-	3	1.802-	2	2.534-	3	0.830-	3	1.673-	2
17	2.268-	4	1.355-	2	1.160-	2	7.776-	4	1.650-	2	5.979-	3	1.154-	3	1.732-	2	1.794-	3
18	5.753-	3	1.633-	2	4.633-	4	1.203-	2	1.065-	2	8.103-	4	1.572-	2	6.758-	3	5.251-	3
19	1.515-	2	5.476-	3	4.670-	3	4.461-	2	3.576-	4	1.131-	2	9.149-	3	1.298-	3	1.494-	2
20	3.139-	3	2.906-	4	4.360-	3	7.142-	4	2.296-	3	3.353-	3	0.398-	5	6.008-	3	1.153-	3
21																	3.0667-	3

Table 61

RK2 FRANCK-COCONON FACTORS FOR H 21

	WV	0	1	2	3	4	5	6	7	8	9	10
1	1.155-	2	3.586-	2	6.626-	2	1.176-	1	1.280-	1	1.261-	1
2	1.4793-	2	1.023-	1	1.193-	1	5.405-	2	1.611-	2	1.351-	4
3	1.011-	1	1.311-	1	7.481-	2	3.025-	3	3.347-	2	5.369-	2
4	1.436-	1	9.025-	2	5.462-	3	6.821-	2	6.833-	2	4.082-	2
5	1.598-	1	2.943-	2	1.538-	2	4.733-	2	2.372-	2	4.428-	4
6	1.506-	1	3.666-	4	5.409-	2	1.605-	3	2.221-	2	5.228-	2
7	1.4233-	1	1.425-	2	8.904-	2	2.862-	2	5.256-	2	1.916-	2
8	9.122-	2	4.874-	2	5.222-	2	5.379-	2	2.245-	2	2.471-	3
9	6.264-	2	7.856-	2	1.587-	2	6.151-	2	6.076-	3	3.615-	2
10	4.078-	2	9.113-	2	1.109-	4	1.113-	4	2.119-	2	3.833-	2
11	2.556-	2	8.757-	2	8.320-	3	1.883-	3	1.260-	2	1.116-	2
12	1.573-	2	7.477-	2	2.793-	2	1.946-	2	3.444-	2	4.308-	4
13	9.629-	3	5.923-	2	6.644-	2	6.867-	2	1.206-	2	1.574-	2
14	3.867-	3	4.626-	2	5.710-	2	5.710-	2	4.730-	2	1.597-	4
15	3.619-	3	3.206-	2	3.960-	2	5.960-	2	3.976-	2	3.172-	2
16	2.253-	3	2.276-	2	5.589-	2	5.569-	2	2.445-	2	1.755-	2
17	1.424-	3	1.586-	2	6.883-	2	1.883-	2	1.846-	2	3.357-	3
18	9.126-	4	1.103-	2	4.053-	2	4.053-	2	2.201-	3	3.795-	2
19	5.977-	4	7.730-	3	3.266-	2	4.265-	2	1.316-	5	3.445-	2
20	3.965-	4	5.376-	3	2.561-	2	2.561-	2	2.114-	3	2.614-	2
21	2.672-	4	3.775-	3	1.974-	2	1.974-	2	6.158-	3	1.695-	2
22	1.759-	4	2.569-	3	1.445-	2	1.445-	2	9.769-	3	6.823-	3
23	9.437-	5	1.411-	3	6.356-	3	6.356-	3	9.015-	3	3.248-	3
24	4.823-	5	7.424-	4	4.657-	3	4.657-	3	5.255-	3	1.864-	2
	3.166-	5	5.607-	4	3.260-	3	3.260-	3	7.895-	3	1.315-	2
											1.816-	3
											2.806-	3
											5.106-	3
											2.755-	3
											4.244-	3

Table 61 (cont'd)

4443 FRANCK-COUDON FACTORS: CCR(1N2 3-M 2)

	11	12	13	14	15	16	17	18	19	20	21
1	3.547-	2	2.241-	2	1.323-	2	7.313-	3	3.753-	6	3.135-
2	3.136-	2	3.424-	2	3.911-	2	2.335-	2	1.072-	2	1.227-
3	2.256-	2	4.648-	2	2.472-	2	1.966-	2	2.425-	3	3.434-
4	2.249-	2	1.425-	2	8.012-	2	6.826-	2	4.917-	2	3.844-
5	1.414-	2	4.309-	2	5.324-	2	1.169-	2	1.142-	2	2.263-
6	4.032-	2	1.649-	2	1.355-	3	2.045-	2	0.997-	2	6.710-
7	2.559-	3	2.055-	2	4.355-	2	2.262-	2	3.337-	2	6.001-
8	3.931-	2	2.445-	2	4.797-	4	1.532-	2	4.004-	2	2.933-
9	9.723-	3	3.764-	3	3.128-	2	3.41-	2	3.575-	3	3.038-
10	9.273-	3	3.355-	2	1.650-	2	4.346-	4	2.396-	2	9.038-
11	3.200-	2	1.067-	2	3.296-	3	2.050-	2	4.344-	2	1.535-
12	1.141-	2	3.526-	3	2.748-	2	1.457-	2	8.253-	4	1.993-
13	1.005-	3	2.472-	2	1.475-	2	1.053-	3	2.309-	2	1.322-
14	2.794-	2	1.005-	2	5.591-	5	1.397-	2	2.650-	4	1.293-
15	2.312-	2	1.568-	3	1.346-	2	1.951-	2	1.152-	4	1.751-
16	9.350-	3	4.479-	3	2.164-	2	2.430-	3	1.016-	2	1.914-
17	6.521-	2	1.710-	2	1.051-	2	2.624-	3	1.999-	2	3.832-
18	5.417-	3	1.045-	2	3.751-	4	1.424-	2	1.125-	2	1.634-
19	1.534-	2	8.066-	3	3.738-	3	1.717-	2	8.312-	4	1.221-
20	1.034-	2	8.582-	4	1.256-	2	8.972-	3	2.499-	3	1.618-
21	1.317-	2	1.215-	3	1.561-	2	1.152-	3	1.032-	2	1.720-
22	5.470-	3	6.426-	3	1.085-	2	6.443-	4	1.305-	2	1.653-
23	9.571-	4	7.715-	3	4.019-	3	3.037-	3	7.816-	3	8.458-
24	1.146-	4	6.916-	3	3.176-	4	5.263-	3	2.425-	3	5.337-

Table 62

RK2 FRANCK-CONDON FACTORS FOR (N2+ HEI1+)

γ	$\nu\nu$	ν	1	2	3	4	5	6	7	8	9	10
1	3.1166-	1	3.646-	1	1.0162-	1	1.652-	2	1.487-	3	7.816-	5
1	3.165-	1	5.256-	2	3.531-	1	2.177-	1	5.306-	2	6.566-	3
2	1.239-	1	2.454-	1	1.334-	2	2.126-	1	2.849-	1	1.042-	1
3	3.753-	2	1.920-	1	1.429-	1	8.883-	2	6.504-	1	2.953-	1
4	1.034-	2	3.196-	2	1.617-	1	1.552-	2	1.515-	1	1.316-	2
5	2.840-	3	3.522-	2	1.320-	1	1.210-	1	2.726-	3	1.592-	1
6	7.599-	4	1.244-	2	6.735-	2	1.400-	1	5.386-	2	3.594-	2
7	2.065-	4	3.899-	3	2.870-	2	9.509-	2	1.166-	1	1.055-	2
8	5.700-	5	1.239-	3	4.110-	2	5.006-	2	1.091-	1	7.591-	2
9	1.654-	5	3.945-	4	4.096-	3	2.294-	2	7.053-	2	1.024-	1
10	4.861-	6	1.274-	4	1.474-	3	9.716-	3	3.815-	2	6.391-	2
11	1.477-	6	4.192-	5	5.299-	4	3.947-	3	1.851-	2	5.370-	2
12	4.0594-	7	1.403-	5	1.918-	4	1.572-	3	0.437-	3	2.983-	2
13	1.479-	7	4.771-	6	7.016-	5	6.225-	4	3.719-	3	1.522-	2
14	4.944-	8	1.647-	6	2.593-	5	2.471-	4	1.602-	3	7.372-	3
15	1.701-	8	5.781-	7	3.664-	6	9.831-	5	6.868-	4	3.465-	3
16	5.876-	9	2.066-	7	3.627-	5	3.965-	5	2.939-	4	1.631-	3
17	1.962-	9	7.493-	8	1.371-	5	1.564-	5	1.258-	4	7.330-	4
18	6.164-14	10	2.723-	8	5.212-	7	6.362-	6	5.355-	5	3.341-	4
19	1.660-14	9	9.700-	9	1.967-	7	2.555-	6	2.301-	5	1.519-	4
20	3.879-14	9	3.279-	9	7.522-	8	1.024-	6	9.799-	6	6.879-	5

Table 62 (cont'd)

(N20 MEINEL)

	VV	11	12	13	14	15	16	17	18	19	20
Y	1.104-11	2.0359-12	1.0341-11	1.0375-12	1.0394-13	3.0552-13	1.0055-12	2.0371-13	1.0014-14	0.502-14	
1	1.0343-11	1.0474-13	2.0123-11	1.0789-11	2.0906-11	2.0373-12	4.0553-12	5.0879-12	7.0656-13	3.0389-13	
2	1.0656-10	1.0398-13	4.0191-11	2.0582-11	2.0916-12	3.0615-11	1.0423-11	2.0719-13	7.0740-12	5.091-12	
3	7.0791-11	9.0719-11	3.0342-12	1.060-10	9.0271-11	1.0012-14	3.0809-11	2.0955-11	7.0747-13	7.0502-12	
4	2.0139-6	1.0395-9	6.0103-12	7.0503-12	5.0660-11	9.0555-11	3.0944-12	2.0354-11	3.0679-11	7.0403-12	
5	0.0744-	1.0377-	3.0146-	3.0406-11	3.0655-12	4.0246-11	9.0356-11	1.0356-11	1.0515-11	4.0765-11	
6	1.0358-	2.0220-	3.0092-	3.0273-	3.0834-12	2.0339-12	2.0179-11	7.0134-11	1.0625-11	0.763-12	
7	2.0350-	1.0352-	2.0037-	3.0636-	3.0833-	3.0345-10	1.0113-14	3.0370-12	4.0492-11	1.0840-11	
8	2.0371-	1.0393-	1.0194-	3.0194-	3.0602-	3.0433-11	1.0539-	3.0380-12	3.0978-13	1.0981-11	
9	2.0128-	3.0293-	1.0209-	4.0713-	3.0676-	2.0219-	3.0994-	3.0574-	2.0273-9	5.0124-11	1.323-11
10	1.0252-	1.0247-	3.0916-	1.0470-	1.0373-	2.0563-	3.0275-	1.0275-	2.0533-	1.021-	1.316-11
11	1.0361-	2.0370-	1.0680-	2.0502-	2.0694-	1.0253-	2.0135-	3.0135-	3.0746-	4.0617-	1.0845-
12	2.0325-	2.0247-	2.0977-	2.0934-	2.0112-	2.0337-	1.0127-	1.0127-	1.0130-	2.0296-	4.0262-
13	7.0312-	2.0233-	3.00523-	2.05079-	2.0333-	2.0464-	2.0919-	1.0339-	1.0339-	1.0518-	2.0691-
14	4.0312-	2.0315-	2.06397-	3.07835-	2.0598-	2.0535-	2.0535-	2.0535-	2.0939-	1.0557-	1.065-
15	5.0243-	3.0777-	2.0966-	2.0305-	3.0347-	2.0329-	3.0115-	1.0115-	2.0312-	2.0304-	1.0777-
16	4.0120-	3.0702-	2.06107-	2.0811-	2.0814-	2.0772-	2.0315-	1.0112-	1.0112-	0.8020-	2.0820-
17	2.0546-	2.0546-	6.0183-	2.0520-	2.0272-	3.0337-	2.0516-	2.0516-	2.076-	3.0115-	1.0581-
18	4.0340-	2.0134-	2.03829-	3.0314-	2.0207-	2.0516-	4.0725-	2.0897-	2.0897-	3.0862-	1.066-
19	4.0355-	2.0335-	2.0497-	3.0299-	2.0856-	2.0609-	2.0609-	2.0609-	3.0622-	3.0223-	1.065-
20	4.0362-	2.0182-	2.0739-	2.0739-	2.0336-	2.0336-	2.0726-	2.0726-	2.0636-	2.0178-	3.0916-

Table 63

RK2 FRANC^E-COURANT FACTORS F_C(N2+ 1ST. VE5.)

	W	0	1	2	3	4	5	6	7	8	9	10
0	6.632-	1	2.053-	1	6.354-	2	1.365-	2	2.921-	3	6.714-	4
1	2.095-	1	2.385-	1	2.056-	1	1.294-	1	4.178-	2	1.138-	2
2	4.451-	2	3.999-	1	5.749-	2	2.289-	1	1.648-	1	7.133-	2
3	2.326-	3	9.934-	2	4.219-	1	2.972-	3	1.535-	1	1.798-	1
4	2.017-	3	6.363-	3	1.607-	1	3.948-	1	4.425-	3	8.794-	2
5	3.119-	5	6.031-	6	1.112-	2	2.107-	1	3.668-	1	1.626-	2
6	6.274-	7	2.267-	5	1.983-	3	1.267-	2	2.532-	1	3.636-	1
7	1.868-	7	1.652-	9	1.166-	4	5.407-	4	9.335-	3	2.711-	1
8	6.661-	8	1.552-	7	7.991-	6	2.395-	4	2.394-	3	3.090-	3
9	1.991-	7	2.410-	10	1.669-	5	1.101-	5	2.100-	4	5.316-	3
10	3.612-	9	4.435-	7	4.256-	10	5.051-	8	6.128-	5	1.975-	5
11	5.245-	11	4.420-	7	9.059-	11	1.995-	5	4.237-	7	2.411-	4
12	7.842-	9	4.969-	6	1.530-	7	1.964-	6	5.244-	6	1.499-	5
13	5.090-	9	3.280-	8	2.524-	7	6.072-	6	1.312-	6	4.346-	5
14	2.000-	3	1.169-	7	5.948-	9	3.469-	9	2.949-	6	4.834-	5
15	1.149-	9	8.702-	6	1.713-	9	2.101-	6	4.931-	6	7.435-	7
16	1.0135-	9	2.666-	5	1.499-	7	2.994-	6	7.123-	6	1.127-	10
17	1.011-	9	1.375-	9	1.951-	7	9.192-	10	3.072-	6	5.636-	5
18	4.775-	11	1.566-	9	1.113-	7	2.986-	6	4.789-	9	5.383-	6
19	2.340-	11	4.343-	9	2.305-	9	1.132-	7	1.276-	11	3.350-	5
20	1.690-	10	3.625-	9	1.924-	10	1.225-	7	2.926-	10	2.275-	9

Table 63 (cont'd)

(N2+ 131. 4E5.0)

V	W	X	Y	11	12	13	14	15	16	17	18	19	20		
0	1.679-	7	1.039-	8	2.0357-	9	3.0692-	9	7.0349-	9	7.0195-11	9	0.153-	9	
1	7.865-	9	4.0235-	6	1.0151-14	5.0337-	9	1.0251-	7	4.0414-	7	3.0546-	9	0.566-	9
2	1.923-	5	2.0213-	6	0.494-	6	3.0322-	9	3.0517-	9	3.0605-	8	9.0117-	9	
3	2.0703-	4	6.0374-	5	1.0343-	3	1.0516-	6	3.0935-	8	7.0339-10	1	4.038-	9	
4	2.077-	3	5.0343-	4	1.0555-	4	3.0834-	5	7.0213-	6	5.0353-	7	1.0312-	9	
5	1.0365-	2	3.0448-	3	1.0361-	3	2.0341-	4	7.0488-	5	1.0382-	5	4.0446-	6	
6	3.0191-	2	1.0313-	2	4.0085-	3	1.0647-	3	4.00936-	4	1.0294-	4	2.0957-	5	
7	6.0769-	2	3.0379-	2	1.0563-	2	6.0309-	3	2.0253-	3	7.0313-	4	2.0112-	4	
8	6.0446-	2	6.0537-	2	3.0997-	2	1.0764-	2	7.0498-	3	2.0616-	3	9.0747-	4	
9	7.0375-	2	7.0377-	2	0.426-	2	3.0616-	2	1.0859-	2	9.0213-	3	3.0315-	3	
10	4.0170-	3	6.0451-	2	5.0364-	2	6.0244-	2	3.0343-	2	1.0852-	2	6.0498-	3	
11	5.0695-	2	1.0373-	2	1.0131-	1	3.0337-	2	5.0312-	2	2.0798-	2	1.0313-	2	
12	4.0256-	1	1.0110-	1	4.0396-	2	1.0658-	1	1.0353-	2	2.0043-	2	1.0343-	2	
13	7.0763-	2	2.0213-	1	1.0367-	1	6.008-	2	2.0333-	1	3.0323-	1	6.0393-	2	
14	5.0636-	2	2.0216-	1	4.0779-	2	9.0094-	2	5.0547-	2	3.0396-	1	6.0250-	3	
15	6.0364-	2	5.0325-	4	2.0834-	1	1.0256-	3	2.0675-	2	3.0050-	2	3.0336-	1	
16	1.0113-	2	6.0111-	2	5.0355-	2	1.0878-	1	4.0421-	2	3.0495-	3	4.0357-	4	
17	1.0390-	3	5.0232-	2	2.0105-	2	1.0728-	1	4.0657-	2	3.0431-	2	1.0559-	2	
18	7.0284-	3	4.0281-	3	7.0425-	2	7.0498-	3	2.0311-	1	5.0854-	3	2.0850-	2	
19	3.0666-	3	2.0381-	3	3.0616-	2	3.0295-	2	3.0325-	2	3.0306-	2	3.0279-	2	
20	4.0968-	4	3.0268-	3	3.0665-	3	2.0922-	2	3.0313-	4	1.0349-	1	6.0773-	3	

Table 64

TABLE FRANCK-COUDJN FACTORS FOR N2O AND NO.

v	v	a	1	2	3	4	5	6	7	8	9	10
1	1.317-	2	7.594-	2	1.916-	1	2.461-	1	1.398-	1	4.039-	2
1	4.864-	2	1.565-	1	1.568-	1	2.726-	2	3.181-	2	1.082-	1
2	9.626-	2	1.530-	1	2.608-	2	3.801-	2	1.177-	1	2.833-	2
3	1.354-	1	0.345-	2	7.956-	3	9.608-	2	1.269-	2	5.568-	2
4	1.517-	1	1.921-	2	6.118-	2	4.219-	2	2.461-	2	6.895-	2
5	1.644-	1	1.732-	4	6.160-	2	1.641-	4	6.893-	2	3.072-	3
6	1.217-	1	1.862-	2	2.308-	2	2.367-	2	3.927-	2	2.337-	2
7	9.342-	2	4.036-	2	1.579-	2	5.504-	2	2.408-	3	5.443-	2
8	6.668-	2	6.894-	2	1.382-	4	5.474-	2	9.301-	3	3.360-	2
9	4.540-	2	7.519-	2	7.384-	3	3.094-	2	3.524-	2	4.116-	3
10	2.953-	2	6.936-	2	2.617-	2	6.446-	3	4.553-	2	4.856-	2

v	v	11	12	13	14	15	16	17	18	19	20	21
0	2.989-	7	3.0233-	6	4.612-	9	7.976-	10	7.902-	11	3.937-	11
1	2.136-	5	7.948-	7	3.167-	7	1.709-	6	9.767-	9	1.392-	10
2	1.421-	6	7.215-	5	1.098-	0	1.505-	6	1.811-	6	2.297-	6
3	1.117-	2	3.417-	6	1.756-	4	5.262-	7	4.699-	5	2.655-	10
4	1.452-	1	1.379-	2	5.965-	5	3.435-	4	1.391-	7	1.753-	7
5	2.719-	1	1.954-	1	2.271-	2	2.123-	4	5.711-	4	5.956-	5
6	1.261-	2	2.614-	1	2.062-	1	3.740-	4	8.349-	4	3.114-	5
7	7.281-	2	9.459-	4	2.637-	1	3.635-	2	1.213-	3	1.689-	3
8	4.662-	3	6.242-	2	1.351-	3	2.203-	1	2.993-	1	3.937-	2
9	2.718-	2	1.985-	2	4.478-	2	9.254-	3	1.923-	1	3.335-	1
10	3.989-	2	7.051-	3	3.289-	2	2.612-	2	1.758-	1	3.652-	1

Table 65

TABLE 65 FRANCK-CODDINGTON FACTORS = J2 (NO 344A (1/2))

V	V	W	U	1	2	3	4	5	6	7	8	9	10	11	
1 1.615-1	2 0.611-1	2 0.397-1	1 0.014-1	9.0156-2	4.0393-2	2.0234-2	9.0654-3	3.0392-3	1.0338-3	5.097-4	2.0320-4				
1 3.322-1	4 0.73-1	5 0.730-4	7 0.312-2	1.0302-1	1.317-1	3.0318-2	5.0197-2	3.0396-2	1.0702-2	6.0120-3	3.0789-3				
2 2.927-1	1 0.423-2	1 0.544-1	7 0.324-2	5.0478-4	3.0333-2	5.0552-2	1.047-1	6.0998-2	6.0329-2	3.0499-2	2.0289-2				
3 1.551-1	4 0.93-1	4 0.735-2	3 0.773-2	1.0115-1	5.0444-2	7.0593-4	2.0133-2	6.0297-2	8.0344-2	7.0901-2	0.0211-2				
4 5.043-2	2 0.413-1	4 0.55-2	1 0.235-1	2.0436-3	2.0444-2	8.0732-2	3.0443-2	2.0436-4	1.0721-2	4.0367-2	0.0987-2				
5 1.100-2	1 0.34-1	2 0.161-1	6 0.322-4	1.0099-1	4.0750-2	4.0139-3	6.0275-2	5.0733-2	2.0135-2	1.0441-7	1.0377-2				
V	V	W	U	12	13	14	15	16	17	18	19	20	21	22	23
1 9.034-5	3 0.667-2	1 0.585-5	7 0.448-6	3.0749-5	1.0455-6	9.0013-7	2.0473-7	2.0520-8	9.0361-9	6.0653-8	1.0155-7				
2 1.705-3	7 0.57-4	3 0.397-4	2 0.539-4	6.0976-5	2.0394-5	1.0158-5	3.0955-5	1.0054-5	1.0374-7	9.0943-9	3.0850-9				
2 1.224-2	2 0.183-3	3 0.010-3	1 0.431-3	6.0735-4	3.0053-4	1.0377-4	5.0955-5	2.0437-5	9.0239-6	3.0144-6	0.0744-7				
3 4.200-2	2 0.55-2	1 0.451-2	7 0.477-3	4.0161-3	2.0111-3	1.0032-3	4.0399-4	2.0273-4	1.0223-4	4.0494-5	4.0421-5				
4 6.969-2	3 0.652-2	4 0.416-2	2 0.616-2	1.0597-2	9.0234-3	5.0176-3	2.0725-3	1.0371-3	6.067-4	3.0296-4	1.0342-4				
5 4.230-2	3 0.894-2	5 0.030-2	3 0.035-2	3.0859-2	2.0041-2	1.0356-2	1.0032-2	5.0639-3	3.0155-3	1.0722-3	9.0183-4				

Table 66

RK2 FRANCK-CONDON FACTORS = 32 (NO GAIA (3/2))

V	V'	0	1	2	3	4	5	6	7	8	9	10	11	
0	1.511-	1	2.516-	1	2.346-	1	1.674-	1	9.994-	2	5.235-	2	2.427-	2
1	3.261-	1	4.266-	1	7.061-	1	5.858-	2	1.243-	1	1.316-	1	1.021-	1
2	2.975-	1	9.639-	3	1.454-	1	8.214-	2	2.465-	3	2.526-	2	7.035-	2
3	1.566-	1	1.869-	1	3.718-	2	2.708-	2	1.076-	1	5.826-	2	2.779-	3
4	5.370-	2	2.449-	1	3.379-	2	1.237-	1	5.332-	3	4.619-	2	1.520-	2
5	1.248-	2	1.492-	1	3.834-	3	9.341-	2	5.488-	2	1.370-	2	1.131-	2
									1.337-	3	5.474-	2	1.198-	2
									1.337-	3	5.474-	2	1.198-	2
									1.337-	3	5.474-	2	1.198-	2
									1.337-	3	5.474-	2	1.198-	2

V	V'	12	13	14	15	16	17	18	19	20	21	22	23	
0	1.196-	4	5.251-	3	2.346-	5	9.528-	6	3.538-	6	1.125-	6	2.792-	7
1	1.966-	3	6.810-	4	3.909-	4	1.766-	4	8.811-	5	3.439-	5	1.399-	5
2	1.361-	2	6.996-	3	3.467-	3	1.660-	3	7.737-	4	3.561-	4	1.658-	4
3	6.490-	2	2.821-	2	1.646-	2	6.995-	3	4.698-	3	2.392-	3	1.174-	3
4	6.981-	2	5.926-	2	4.368-	2	2.876-	2	1.756-	2	1.020-	2	5.646-	3
5	3.753-	2	5.663-	2	6.436-	2	5.333-	2	4.033-	2	2.833-	2	1.024-	2
									4.033-	2	2.833-	2	1.024-	2
									4.033-	2	2.833-	2	1.024-	2
									4.033-	2	2.833-	2	1.024-	2
									4.033-	2	2.833-	2	1.024-	2

Table 67

RK2 FRANCK-COMDON FACTORS FJ2 (NO BETA (1/2))

VV	0	1	2	3	4	5	6	7	8	9	10	11
1	1.709-5	2.0473-4	1.671-3	7.411-3	2.312-2	5.344-2	3.772-2	1.438-1	1.714-1	1.703-1	1.444-1	9.467-2
2	1.451-4	1.682-3	9.120-3	3.197-2	7.019-2	1.073-1	1.120-1	7.112-2	1.635-2	2.350-3	4.666-2	1.~88-1
3	6.172-4	2.692-3	2.552-2	6.380-2	9.716-2	8.240-2	2.916-2	2.245-4	3.649-2	6.946-2	6.325-2	1.106-2
4	1.040-3	1.433-2	6.740-2	8.048-2	7.607-2	2.081-2	2.801-3	4.697-2	6.353-2	1.963-2	4.234-3	5.354-2
5	4.330-3	2.721-2	6.760-2	7.931-2	2.930-2	8.457-4	4.127-2	5.349-2	9.101-3	1.417-2	5.783-2	3.311-2
6	1.402-2	2.714-2	6.991-2	1.062-2	7.451-3	4.0779-2	2.046-2	4.703-3	4.392-2	1.301-2	5.930-3	4.503-2
7	2.225-2	6.755-2	5.117-2	1.047-3	3.006-2	3.727-2	3.722-5	3.215-2	2.740-2	1.278-3	3.817-2	1.771-2
8	3.161-2	7.062-2	2.605-2	4.059-3	4.311-2	1.195-2	1.242-2	3.659-2	1.253-3	2.073-2	2.451-2	2.339-3
9	4.093-2	6.582-2	9.406-3	1.984-2	3.636-2	1.326-5	3.171-2	1.467-2	9.296-3	3.275-2	3.356-4	2.098-2
10	4.925-2	2.506-2	6.024-4	3.320-2	1.950-2	1.630-2	8.395-3	3.237-2	1.153-4	2.893-2	1.153-2	1.311-2
11	5.672-2	4.065-2	1.663-3	3.632-2	3.626-3	2.391-2	1.536-2	1.299-3	2.749-2	2.263-4	2.926-2	3.494-3
12	6.247-2	2.613-2	1.013-2	3.323-2	3.294-4	3.139-2	2.194-3	2.351-2	1.012-2	1.343-2	1.928-2	4.472-3
13	6.617-2	1.363-2	2.369-2	2.156-2	7.403-3	2.585-2	1.493-3	2.715-2	3.963-5	2.575-2	2.303-3	2.152-2
14	6.794-2	4.917-3	2.977-2	9.545-3	1.820-2	1.334-2	1.136-2	1.705-2	6.432-3	2.161-2	2.806-3	2.305-2
15	6.821-2	5.654-4	3.444-4	1.752-3	2.574-2	2.329-3	2.142-2	4.572-3	1.646-2	6.656-3	1.564-2	6.019-3
16	6.659-2	4.300-4	3.389-2	1.972-4	2.637-2	1.238-4	2.356-2	2.878-3	2.256-2	2.072-7	2.192-2	3.322-5
17	6.366-2	3.864-3	2.902-2	4.236-3	2.076-2	4.042-3	1.758-2	5.045-3	1.616-2	5.455-3	1.505-2	2.368-3
18	5.927-2	9.821-3	2.133-2	1.147-2	1.234-2	1.230-2	9.051-3	1.370-2	5.793-3	1.582-2	4.921-3	1.625-2
19	5.389-2	1.711-2	1.302-2	1.659-2	4.268-3	1.924-2	1.259-3	1.881-2	1.671-4	1.981-2	6.371-5	1.817-2

Table 67 (cont'd)
(NO BETA (1/2))

	VV	12	13	14	15	16	17	18	19	20	21	22	23
1	5.375-2	2.59/-2	1.050-2	3.489-3	8.933-4	1.717-4	2.834-5	5.877-5	8.197-7	1.120-8	1.770-8	2.469-8	
2	1.413-1	4.270-1	8.577-2	4.448-2	1.771-2	5.591-3	1.415-3	2.691-4	4.143-5	3.967-6	1.122-9	6.264-9	
3	7.912-3	6.663-2	1.261-1	1.337-1	9.468-2	4.099-2	1.919-2	5.549-3	1.187-3	1.753-4	1.502-5	3.337-7	
4	7.215-2	2.533-2	1.635-3	5.634-2	1.220-1	1.326-1	3.238-2	4.391-2	1.498-2	3.577-3	5.559-4	4.829-5	
5	1.166-4	4.144-2	7.100-2	2.534-2	2.699-3	6.403-2	1.314-1	1.278-1	7.777-2	3.152-2	8.195-3	1.311-3	
6	1.891-2	9.027-3	5.362-2	2.629-2	3.135-3	5.665-2	3.439-2	2.073-3	3.997-2	1.305-1	1.414-1	8.163-2	
7	6.810-3	4.434-2	1.175-2	1.381-2	5.187-2	1.155-2	1.655-2	6.795-2	2.858-2	6.194-3	9.555-2	1.565-1	
8	3.827-2	1.063-2	1.400-2	4.138-2	2.177-3	2.973-2	4.396-2	1.865-4	4.497-2	5.887-2	1.492-3	5.592-2	
9	1.703-2	7.287-3	3.666-2	1.929-3	2.797-2	2.033-2	1.920-3	4.679-2	1.874-2	1.306-2	6.784-2	1.929-2	
10	6.005-4	3.265-2	9.197-3	1.957-2	2.716-2	1.747-3	4.070-2	8.382-3	2.199-2	4.328-2	2.784-8	2.337-2	
11	2.114-2	1.666-2	7.476-3	2.997-2	1.490-5	3.261-2	9.712-3	1.895-2	3.192-2	1.261-3	4.737-2	1.058-2	
12	2.716-2	1.959-5	2.845-2	3.587-3	2.233-2	1.531-2	1.021-2	3.049-2	5.806-4	3.948-2	5.022-3	3.047-2	
13	8.061-3	1.471-2	1.622-2	7.356-3	2.441-2	1.403-3	3.097-2	4.525-4	2.996-2	7.352-3	2.293-2	2.311-2	
14	4.884-4	2.480-2	1.505-4	2.471-2	2.195-3	2.244-2	7.192-3	1.795-2	1.535-2	1.121-2	2.520-2	4.467-3	
15	1.274-2	4.214-2	9.599-3	1.558-2	6.744-3	1.979-2	3.717-3	2.416-2	1.229-3	2.777-2	6.231-5	3.119-2	
16	2.168-2	2.403-4	2.157-2	6.540-4	2.168-2	1.490-3	2.150-2	2.775-3	2.139-2	4.556-3	2.135-2	7.102-3	
17	1.470-2	5.955-3	1.463-2	5.981-3	1.514-2	5.169-3	1.511-2	5.891-3	1.753-2	5.889-3	1.880-2	6.071-3	
18	2.070-3	1.703-2	2.056-3	1.789-2	1.371-3	1.690-2	3.033-4	2.023-2	6.749-4	2.157-2	2.332-2	2.709-4	
19	6.841-4	1.721-2	1.820-3	1.590-2	3.436-3	1.434-2	3.144-3	1.326-2	7.439-3	1.144-2	1.068-2	9.306-3	

Table 68
R&R FRANC<-COUNON FACTORS FOR (453614 (3/21))

	11	10	9	8	7	6	5	4	3	2	1	0	11	
1	1.910-	2	2.634-	1	1.635-	3	7.930-	3	2.420-	2	5.023-	2	1.408-	1
2	1.559-	4	1.816-	3	3.933-	3	3.274-	2	1.039-	2	1.115-	1	1.713-	1
3	0.994-	4	3.345-	3	2.727-	2	0.609-	2	9.699-	2	2.047-	2	1.126-	1
4	1.956-	3	1.519-	2	3.133-	2	9.537-	2	7.292-	2	6.142-	2	5.992-	4
5	4.582-	3	2.836-	2	7.468-	2	7.762-	2	2.630-	2	1.828-	2	4.079-	3
6	1.376-	3	4.427-	2	7.657-	2	4.639-	2	6.770-	4	2.345-	2	5.914-	2
7	1.533-	2	5.077-	2	7.044-	2	1.536-	2	9.556-	3	4.655-	2	5.162-	2
8	2.355-	2	3.608-	2	6.362-	2	3.895-	4	3.260-	2	3.512-	2	4.452-	2
9	3.286-	2	7.033-	2	2.575-	2	2.740-	3	6.355-	2	9.682-	3	1.521-	2
10	4.230-	2	6.523-	2	7.637-	3	2.171-	2	3.466-	2	7.731-	5	3.362-	2
11	5.116-	2	2.371-	2	1.943-	4	3.546-	2	1.610-	2	1.039-	2	3.033-	6
12	5.834-	2	3.697-	2	2.946-	3	3.881-	2	2.376-	3	2.556-	2	1.056-	2
13	6.401-	2	2.428-	2	1.222-	2	3.182-	2	9.189-	4	3.130-	2	1.095-	3
14	6.752-	2	1.248-	2	2.346-	2	1.919-	2	9.442-	3	2.497-	2	2.710-	3
15	6.903-	2	3.917-	3	3.138-	2	7.361-	3	2.826-	2	1.121-	2	1.366-	2
16	0.896-	2	2.497-	4	3.469-	2	7.980-	4	2.691-	2	1.801-	3	2.284-	2
17	6.697-	2	6.347-	4	3.317-	2	7.980-	4	2.599-	2	5.217-	4	3.635-	4
18	5.869-	2	1.462-	2	1.924-	2	1.385-	2	1.015-	2	6.891-	3	6.334-	2
19	5.319-	2	1.905-	2	1.039-	2	2.0494-	2	2.942-	3	2.037-	2	3.259-	4

Table 68 (cont'd)

(VO BETA (3/2))

V	VV	12	13	14	15	16	17	18	19	20	21	22	23	
1	5.192-	2	2.453-	2	9.712-	3	3.173-	3	8.217-	4	1.621-	4	2.223-	6
2	1.425-	1	1.251-	1	8.173-	2	6.187-	2	1.696-	2	5.246-	3	1.265-	3
3	1.001-	2	7.156-	2	1.260-	1	1.317-	1	9.261-	2	4.651-	2	1.778-	2
4	7.191-	2	2.190-	2	2.973-	3	5.995-	2	1.259-	1	1.396-	1	1.138-	2
5	5.933-	4	4.535-	2	6.937-	2	2.136-	2	6.328-	3	6.339-	2	1.325-	1
6	5.250-	2	3.123-	2	7.318-	4	4.818-	2	6.533-	2	1.192-	2	1.491-	2
7	1.640-	2	6.458-	3	5.163-	2	2.392-	2	4.931-	3	5.357-	2	3.153-	2
8	9.332-	3	4.673-	2	9.229-	3	1.662-	2	5.176-	2	6.874-	3	2.826-	2
9	3.871-	2	6.274-	3	1.697-	2	4.634-	2	1.056-	3	3.324-	2	4.039-	2
10	1.432-	2	9.726-	3	3.534-	2	9.429-	4	3.974-	2	2.626-	2	3.428-	3
11	1.456-	3	3.320-	2	4.311-	3	2.198-	2	2.470-	2	3.234-	3	6.157-	2
12	2.314-	2	1.395-	2	3.708-	3	2.856-	2	3.292-	4	3.414-	2	5.243-	3
13	2.576-	2	3.757-	4	2.910-	2	2.255-	3	2.437-	2	1.278-	2	2.832-	2
14	6.087-	3	1.699-	2	1.397-	2	3.309-	3	2.248-	2	2.764-	3	3.978-	2
15	1.249-	3	2.434-	2	4.616-	6	2.526-	2	1.116-	3	2.431-	2	5.326-	3
16	1.473-	2	9.885-	3	1.177-	2	1.378-	2	8.614-	3	1.758-	2	5.412-	3
17	2.180-	2	2.191-	2	2.133-	2	1.713-	4	2.211-	2	5.937-	4	2.271-	2
18	1.291-	2	7.783-	3	1.289-	2	7.735-	3	1.326-	2	7.876-	3	1.432-	2
19	1.701-	3	1.612-	2	1.023-	3	1.884-	2	6.043-	4	1.959-	2	3.394-	4
20	1.517-	3	1.613-	2	3.051-	3	1.463-	2	6.006-	3	1.292-	2	6.901-	3

Table 69

TABLE FRANCK-CONDON FACTORS FOR NO₂ DE-TA (11/21)

V	VV	0	1	2	3	4	5	6	7	8	9	10	11
1	1.619-1	2.019-1	2.405-1	1.020-1	9.149-2	4.026-2	2.124-2	3.055-3	3.412-3	1.219-3	4.150-4	1.357-4	
1	3.438-1	1.032-1	1.499-3	7.544-2	1.334-1	1.303-1	3.547-2	5.729-2	2.970-2	1.384-2	5.964-3	2.427-3	
2	3.041-1	2.570-2	1.510-1	6.049-2	1.535-4	4.495-2	9.706-2	1.055-1	6.457-2	5.468-2	3.097-2	1.590-2	
3	1.410-1	2.405-1	2.553-2	6.282-2	1.096-1	3.141-2	1.327-3	3.939-2	9.037-2	8.447-2	7.292-2	2.001-2	
4	3.757-2	2.46,-1	9.756-2	9.332-2	2.755-3	6.148-2	7.179-2	1.093-2	5.934-3	4.279-2	7.227-2	7.734-2	
V	VV	12	13	14	15	16	17	18	19	20	21	22	23
1	4.0132-5	1.196-5	3.367-6	9.746-7	2.944-7	7.711-8	5.448-9	9.033-9	6.253-8	1.322-7	1.759-7	1.326-7	
1	9.113-4	3.203-4	1.067-4	3.206-5	6.392-5	1.273-6	2.310-9	3.156-7	7.031-7	7.985-7	6.444-7	4.123-7	
2	7.364-3	3.061-3	2.175-3	4.032-4	1.223-4	2.692-5	3.973-6	7.935-3	8.084-7	1.729-0	1.967-6	1.659-6	
3	2.924-2	1.501-2	6.955-3	2.929-3	1.215-3	3.641-4	3.483-5	1.620-5	3.124-7	1.125-6	3.343-6	4.432-6	
4	6.276-2	4.190-2	2.429-2	1.256-2	5.034-3	2.455-3	6.894-4	2.659-4	5.448-5	3.957-6	1.171-6	6.561-6	

Table 70

RK2 FRANCK-CONDON FACTORS F_{J2} (NO DELTA (3/2))

VV	0	1	2	3	4	5	6	7	8	9	10	11
Y	1.524-1	2.524-1	2.354-1	1.66J-1	9.995-2	5.145-2	2.374-2	9.985-3	3.661-3	1.44J-3	4.947-4	1.723-4
1	3.427-1	1.125-1	1.6J4-4	6.357-2	1.279-1	1.314-1	3.898-2	6.151-2	3.315-2	1.598-2	7.056-3	2.879-3
2	3.098-1	1.934-2	1.244-1	6.998-2	2.113-4	3.611-2	8.934-2	1.055-1	6.028-2	5.951-2	3.466-2	1.798-2
3	4.478-1	2.335-1	3.359-2	4.989-2	1.393-1	3.648-2	3.650-5	3.202-2	7.443-2	6.814-2	7.582-2	3.323-2
4	6.024-2	2.543-1	6.399-2	1.087-1	5.568-4	7.263-2	7.356-2	1.633-2	2.699-3	3.549-2	6.785-2	7.664-2

VV	12	13	14	15	16	17	18	19	20	21	22	23
Y	6.021-5	2.075-5	6.566-6	1.599-6	1.839-7	5.692-9	1.179-7	1.690-7	1.452-7	0.807-8	4.115-8	1.573-8
1	1.095-3	3.922-4	1.325-4	4.0J93-5	1.0J62-5	1.312-6	3.950-6	2.473-7	7.347-7	9.389-7	6.240-7	3.596-7
2	6.437-3	3.617-3	1.420-3	5.0J20-4	1.576-4	4.0J50-5	7.0223-6	2.119-7	6.626-7	2.153-9	2.843-6	2.623-6
3	3.213-2	1.710-2	3.242-3	3.535-3	1.355-3	4.0J59-4	1.237-6	2.239-5	1.032-5	1.364-6	4.033-6	5.476-6
4	6.511-2	1.56J-2	2.757-2	1.453-2	6.870-3	2.903-3	1.0J58-3	3.253-4	7.211-5	6.461-6	6.609-7	6.374-6

Table 71

TABLE 71
FRANCK-COURN FACTORS FOR (NO₂EP₁₁-Cl₁₁) (11/2)

v	vv	jj	i	2	3	4	5	6	7	8	9	10	11
1.620- 1	2.512- 1	2.312- 1	2.076J- 4	1.071- 1	1.076J- 4	6.499- 2	1.533- 1	9.266- 2	4.946- 2	2.463- 2	1.132- 2	5.177- 3	6.994- 4
3.365- 1	1.071- 1	1.076J- 4	1.076J- 4	1.076J- 4	1.076J- 4	1.228- 1	1.272- 1	3.690- 2	5.434- 2	3.703- 2	1.956- 2	9.641- 3	4.010- 3
2.393- 1	1.045- 2	1.045- 2	1.045- 2	1.045- 2	1.045- 2	7.369- 2	8.897- 4	7.969- 2	9.622- 2	6.309- 2	4.616- 2	4.616- 2	2.033- 2
1.453- 1	2.113- 1	2.113- 1	2.231- 1	2.231- 1	2.231- 1	4.651- 2	1.142- 1	4.944- 2	7.178- 2	1.995- 2	5.962- 2	7.881- 2	7.292- 2
4.396- 2	2.389- 4	2.389- 4	2.193- 2	2.193- 2	2.193- 2	1.343- 1	4.956- 4	6.619- 2	6.726- 2	2.394- 2	5.754- 2	1.921- 2	6.654- 2
9.195- 3	1.196- 4	1.196- 4	2.011- 1	2.011- 1	2.011- 1	6.692- 4	1.255- 4	4.215- 2	9.536- 3	7.250- 2	6.523- 2	1.746- 2	2.743- 2
1.584- 3	3.616- 2	3.616- 2	1.730- 1	1.730- 1	1.730- 1	5.436- 2	5.259- 2	3.925- 2	5.321- 2	3.094- 2	7.092- 2	4.912- 2	4.912- 2
2.809- 4	1.916- 3	1.916- 3	5.034- 2	5.034- 2	5.034- 2	1.931- 1	1.975- 2	2.173- 1	1.939- 3	3.750- 2	4.564- 2	1.677- 3	4.726- 2

v	vv	12	13	14	15	16	17	18	19	20	21	22	23
1.408- 4	5.336- 2	2.0555- 5	6.376- 6	3.646- 6	3.646- 6	1.567- 6	3.756- 6	1.291- 7	9.738- 10	4.359- 6	1.202- 7	1.036- 7	
2.225- 3	9.877- 4	4.244- 4	1.763- 4	7.619- 4	2.233- 5	6.363- 5	1.964- 5	2.334- 5	1.353- 7	1.356- 7	2.735- 7	2.735- 7	
1.339- 2	6.959- 3	3.334- 3	1.546- 3	6.546- 3	2.927- 4	1.362- 4	3.522- 4	1.294- 4	1.417- 6	1.417- 6	4.842- 7	4.842- 7	
4.131- 2	2.546- 2	1.6420- 2	7.774- 3	3.950- 3	1.839- 3	6.298- 3	3.331- 4	1.162- 4	3.064- 5	4.521- 6	3.970- 9	3.970- 9	
6.758- 2	5.432- 2	3.833- 2	2.455- 2	1.464- 2	8.066- 3	4.065- 3	1.038- 3	7.815- 4	2.750- 6	7.242- 5	8.653- 6	8.653- 6	
4.716- 2	5.161- 2	6.017- 2	4.923- 2	3.501- 2	2.329- 2	1.365- 2	7.301- 3	3.536- 3	1.529- 3	5.911- 4	1.559- 4	1.559- 4	
1.865- 3	2.268- 2	4.650- 2	5.747- 2	5.635- 2	3.223- 2	2.039- 2	1.170- 2	5.998- 3	2.737- 3	4.665- 3	4.665- 3	4.665- 3	
2.998- 2	2.463- 3	5.119- 3	2.682- 2	6.794- 2	5.658- 2	5.168- 2	6.076- 2	2.731- 2	1.721- 2	9.646- 3	4.715- 3	4.715- 3	

Table 72

RK2 FRANCK-CONDON FACTORS FOR NO EPSILCN (3/21)

v	v'	u	l	2	3	4	5	6	7	8	9	10	11
1	1·526-1	2·48J-1	2·292-1	1·646-1	1·036-1	5·446-2	2·718-2	1·275-2	5·690-3	2·452-3	1·040-3	4·368-4	
1	3·323-1	1·16J-1	1·114-5	5·396-2	1·169-1	1·257-1	1·016-1	6·816-2	4·049-2	2·292-2	1·126-2	5·479-3	
2	3·035-1	1·393-2	1·515-1	6·259-2	2·999-3	2·161-2	7·121-2	9·559-2	8·914-2	6·725-2	4·443-2	2·065-2	
3	2·526-1	2·J3+1	5·425-2	3·463-2	1·110-1	5·036-2	2·635-3	1·419-2	5·275-2	7·636-2	7·652-2	6·228-2	
4	4·695-2	2·433-1	4·127-2	1·355-1	2·621-3	5·590-2	5·728-2	3·766-2	1·029-3	1·296-2	4·432-2	6·560-2	
5	9·913-3	1·24J-1	2·065-1	3·5J0-3	1·172-1	5·369-2	4·730-3	6·494-2	6·620-2	2·307-2	5·673-5	1·431-2	
6	1·670-3	3·669-2	1·666-1	9·517-2	6·6J2-2	4·115-2	1·024-1	1·020-2	2·254-2	6·685-2	5·064-2	1·259-2	
7	2·938-4	3·695-3	8·795-2	1·093-1	1·224-2	1·211-1	3·813-3	9·035-2	5·458-2	1·117-4	3·946-2	6·185-2	
v	v'	u	l	12	13	14	15	16	17	18	19	20	21
1	1·822-4	7·542-5	2·986-5	1·097-5	3·549-6	9·303-7	1·355-7	6·175-3	5·431-9	1·661-8	1·855-8	1·682-8	
1	2·555-3	1·151-3	5·018-4	2·092-4	8·314-5	3·097-5	1·036-5	2·528-5	3·233-7	5·199-9	1·099-7	3·748-7	
2	1·481-2	7·742-3	3·047-3	1·905-3	8·056-4	3·421-4	1·327-4	4·513-5	1·215-5	1·655-6	1·117-6	8·756-7	
3	4·404-2	2·003-2	1·643-2	8·099-3	4·517-3	2·174-3	3·577-4	3·924-4	1·397-4	3·913-5	5·530-6	1·946-6	
4	6·775-2	2·704-2	4·175-2	2·720-2	1·618-2	8·968-3	4·611-3	2·159-3	9·321-4	3·393-4	9·446-5	1·351-5	
5	4·130-2	5·971-2	6·160-2	5·187-2	3·801-2	2·525-2	1·518-2	8·307-3	4·171-3	1·846-3	6·926-4	1·974-4	
6	4·106-4	1·752-2	4·238-2	5·607-2	5·667-2	4·741-2	3·471-2	2·270-2	1·346-2	7·384-3	3·250-3	1·262-3	
7	3·501-2	5·133-3	2·035-3	2·199-2	4·391-2	5·518-2	3·337-2	4·322-2	3·098-2	1·953-2	1·097-2	5·391-3	

Table 73
2022 FRANCE-CANADA FACTORS : 2022-2023 (1/2)

y	0	1	2	3	4	5	6	7	8	9	10	11
1	2.021- 1	6.723- 2	1.737- 1	2.362- 1	2.164- 1	1.433- 1	7.379- 2	3.032- 2	9.037- 3	2.593- 3	5.636- 4	9.723- 5
2	6.573- 2	1.616- 1	1.373- 1	2.977- 2	9.902- 3	1.019- 1	1.742- 1	1.532- 1	9.532- 1	4.356- 2	1.506- 2	3.926- 3
3	1.165- 1	1.375- 1	1.035- 2	3.120- 2	1.134- 1	5.339- 2	1.129- 4	5.311- 4	1.503- 2	1.536- 1	9.824- 2	4.313- 2
4	1.305- 1	0.146- 2	1.177- 2	3.169- 2	2.892- 2	1.643- 2	3.0275- 2	3.275- 2	9.678- 2	6.426- 2	1.405- 1	1.019- 1
5	1.392- 1	7.729- 3	5.431- 2	4.595- 2	9.315- 3	7.716- 2	1.939- 2	2.124- 2	8.714- 2	3.845- 2	2.941- 3	7.959- 2
6	1.453- 1	4.446- 3	7.389- 2	8.095- 4	6.016- 2	2.447- 2	1.969- 2	5.021- 2	5.996- 3	3.760- 2	6.117- 2	1.633- 2
y	10	11	12	13	14	15	16	17	18	19	20	21
1	1.496- 5	1.217- 0	3.377- 0	9.940- 9	5.363- 8	3.892- 8	1.073- 9	3.733- 8	8.714- 1	2.411- 8	3.372- 9	6.397- 9
2	7.978- 4	1.340- 4	2.087- 5	3.463- 6	3.268- 7	2.416- 8	2.764- 8	6.516- 8	1.050- 8	6.250- 8	3.801- 8	3.249- 8
3	1.419- 2	3.648- 5	7.925- 4	1.370- 4	1.532- 5	6.958- 7	2.589- 8	5.236- 8	2.194- 8	3.991- 9	5.735- 9	1.949- 9
4	5.526- 2	3.734- 2	1.196- 2	2.913- 3	5.278- 4	6.750- 5	5.591- 5	5.953- 7	1.864- 7	3.750- 7	2.739- 4	6.397- 3
5	1.459- 1	1.297- 1	7.250- 2	2.949- 2	8.058- 3	1.718- 3	2.632- 4	3.412- 5	5.214- 6	5.533- 7	6.933- 1	8.937- 3
6	1.446- 1	1.014- 1	1.468- 1	1.116- 1	5.339- 2	1.644- 2	4.732- 3	6.964- 4	1.363- 4	1.933- 5	1.709- 6	8.187- 6

Table 74
R.R FRANCK-COJON FACTORS FOR (40 BETA + 214E (3/2))

VV	8	1	2	3	4	5	6	7	8	9	10	11												
V	2.122-	2	9.086-	2	1.871-	1	2.371-	1	1.439-	1	1.141-	2	2.796-	3	2.676-	3	5.002-	4	9.330-	2				
1	6.961-	2	1.633-	1	1.363-	1	2.516-	2	1.323-	2	1.695-	1	1.757-	1	1.546-	1	9.345-	2	1.423-	2				
2	1.202-	1	1.355-	1	1.099-	2	3.655-	2	1.112-	1	5.208-	2	7.452-	4	7.081-	2	1.522-	1	1.526-	2				
3	1.539-	1	5.740-	2	1.515-	2	3.326-	2	2.420-	2	2.433-	2	3.522-	2	6.837-	2	5.857-	4	6.926-	2				
4	1.612-	1	5.847-	3	6.937-	2	6.104-	2	1.258-	2	7.755-	2	1.345-	2	2.582-	2	8.736-	2	3.408-	2				
5	1.455-	1	6.196-	3	7.947-	2	6.272-	2	2.028-	2	2.463-	2	5.716-	2	3.620-	3	4.195-	2	7.975-	2				
VV	12	13	14	15	16	17	18	19	20	21	22	23												
V	7.161-	6	9.357-	7	6.278-	7	1.291-	6	6.249-	6	6.168-	9	1.803-	9	3.237-10	9	7.352-	9	1.742-11	9	2.869-	9	1.223-	9
1	7.116-	4	1.339-	4	1.307-	5	3.910-	6	5.613-	6	7.707-	6	3.769-	9	3.117-	9	2.656-	9	2.251-	9	1.370-	9	1.534-	11
2	1.332-	2	3.357-	3	6.695-	4	1.129-	4	1.538-	5	6.371-	7	3.371-23	8	3.394-	8	4.193-	9	3.752-	8	1.847-	8	6.247-	3
3	9.362-	2	3.436-	2	1.075-	2	2.566-	3	6.059-	4	6.925-	5	5.098-	6	1.536-	7	1.463-	7	7.928-	6	7.525-	9	3.666-	11
4	1.444-	1	1.266-	1	5.662-	2	2.633-	2	7.508-	3	1.292-	3	2.420-	4	2.610-	5	3.039-	6	1.208-	6	1.263-	7	1.823-	7
5	1.640-	2	1.874-	4	1.460-	1	1.075-	1	5.164-	2	1.710-	2	4.212-	3	7.958-	4	1.226-	4	1.907-	5	2.234-	6	3.155-	10

Table 75
482 FINANCIAL CONDON FACTORS FOR 100% CAPITAL (1/2)

V	IV	6	4	2	3	4	5	6	7	8	9	10	11	
1	1.913-	1	2.795-	1	2.320-	1	1.641-	1	7.795-	2	3.975-	2	6.975-	3
2	3.423-	1	5.061-	2	5.774-	3	9.129-	2	1.411-	1	1.230-	1	2.144J-	4
3	2.753-	1	3.851-	2	1.717-	1	0.215-	2	2.509-	4	4.647-	2	5.434-	3
4	1.366-	1	2.101-	1	2.953-	2	6.079-	2	1.173-	1	9.715-	2	1.511-	2
5	4.371-	2	2.353-	1	3.459-	2	1.136-	1	1.173-	1	3.934-	2	6.359-	2
6	3.981-	3	1.109-	1	6.896-	4	2.221-	1	6.896-	4	7.455-	2	1.911-	2
V	IV	12	13	14	15	16	17	18	19	20	21	22	23	
1	7.060-	5	2.138-	2	3.522-	6	2.339-	5	1.111-	6	6.359-	7	2.195-	7
2	1.382-	3	2.411-	4	2.326-	4	7.427-	5	2.738-	5	1.015-	5	3.219-	5
3	3.974-	3	4.926-	3	2.174-	3	9.243-	4	3.734-	4	1.521-	4	2.191-	5
4	3.520-	2	2.471-	2	1.143-	2	5.975-	3	2.986-	3	1.493-	3	2.278-	4
5	6.729-	2	5.193-	2	3.422-	2	2.163-	2	1.231-	2	7.256-	3	3.044-	3
V	IV	12	13	14	15	16	17	18	19	20	21	22	23	
1	7.060-	5	2.138-	2	3.522-	6	2.339-	5	1.111-	6	6.359-	7	2.195-	7
2	1.382-	3	2.411-	4	2.326-	4	7.427-	5	2.738-	5	1.015-	5	3.219-	5
3	3.974-	3	4.926-	3	2.174-	3	9.243-	4	3.734-	4	1.521-	4	2.191-	5
4	3.520-	2	2.471-	2	1.143-	2	5.975-	3	2.986-	3	1.493-	3	2.278-	4
5	6.729-	2	5.193-	2	3.422-	2	2.163-	2	1.231-	2	7.256-	3	3.044-	3

Table 76

RK2 FRANCK-CONDON FACTORS FOR TWO GAUSS PRIME (3/2)

y	v	w	u	1	2	3	4	5	6	7	8	9	10	11
0	1.698-1	2.703-1	2.287-1	1.505-1	8.563-2	4.417-2	2.146-2	9.933-3	4.346-3	1.803-3	7.138-4	4.791-4		
1	3.371-1	9.531-2	2.444-3	7.880-2	1.368-1	1.303-1	3.654-2	5.684-2	3.332-2	1.715-2	8.363-3	3.014-3		
2	2.810-1	2.352-2	1.644-1	7.219-2	1.334-4	3.749-2	9.351-2	1.041-1	6.720-2	6.030-2	3.724-2	2.112-2		
3	1.630-1	2.093-1	3.730-2	4.765-2	1.162-1	4.581-2	8.520-3	2.621-2	6.778-2	8.451-2	7.642-2	5.729-2		
4	4.656-2	2.353-1	5.310-2	1.200-1	3.663-4	6.465-2	9.587-2	2.753-2	5.881-5	2.279-2	5.572-2	7.185-2		
5	9.574-3	1.223-1	2.191-1	6.136-5	1.104-1	4.085-2	9.113-3	6.921-2	6.336-2	1.600-2	5.376-4	2.0399-2		

y	v	12	13	14	15	16	17	18	19	20	21	22	23
0	9.816-5	3.425-5	1.129-5	3.373-6	6.909-7	2.134-7	5.247-8	2.374-9	2.469-8	3.370-9	4.047-8	4.047-8	3.729-8
1	1.624-3	6.490-4	2.473-4	9.030-5	3.250-5	1.187-5	4.436-6	1.781-5	8.177-7	4.345-7	2.616-7	1.651-7	
2	1.115-2	5.497-3	2.538-3	1.095-3	4.526-4	1.957-4	7.547-5	3.232-5	1.416-5	6.229-6	2.762-6	1.254-6	
3	3.734-2	2.301-2	1.303-2	6.874-3	3.411-3	1.616-3	7.280-4	3.214-4	1.427-4	6.415-5	2.933-5	1.348-5	
4	6.842-2	5.410-2	3.790-2	2.467-2	1.427-2	6.070-3	4.333-3	2.175-3	1.050-3	4.916-4	2.227-4	1.011-4	
5	4.836-2	6.274-2	6.150-2	5.041-2	3.652-2	2.432-2	1.533-2	9.025-3	5.102-3	2.708-3	1.358-3	6.523-4	

Table 77 2x2 FRANC<-CONDON FACTORS FOR (NO + EATM)

v	v	0	1	2	3	4	5					
0	9.996-	1	2.793-	5	1.961-	9	3.971-	5	6.195-	7	1.838-	7
1	2.129-	5	9.976-	1	1.223-	3	2.243-	4	2.255-	4	2.414-	5
2	1.862-	4	1.090-	3	3.943-	1	6.691-	3	4.939-	4	5.535-	4
3	8.556-	2	2.566-	4	3.732-	3	3.711-	1	2.030-	2	6.395-	4
4	5.431-	0	2.701-	4	5.944-	4	1.714-	2	9.334-	1	4.531-	2

Table 78 $\kappa\kappa_2$ FRANCE-FACTORS FOR NO EAST 11

y	0	1	2	3	4	5						
0	9.989-	1	1.136-	4	3.133-	4	1.547-	5	1.541-	5	4.517-	6
1	2.159-	5	9.987-	1	1.107-	4	1.139-	5	4.0791-	5	7.452-	6
2	3.076-	4	1.204-	4	9.934-	1	2.156-	5	4.0115-	4	1.175-	7
3	1.449-	5	4.201-	4	2.244-	2	3.976-	4	5.140-	4	1.929-	6
4	2.184-	6	6.819-	5	4.0122-	4	5.257-	4	9.958-	4	1.614-	3
5	4.745-	6	7.338-	6	2.919-	6	1.637-	4	1.552-	3	9.917-	1
6	1.176-	6	8.656-	6	2.736-	5	2.0352-	5	6.498-	5	1.359-	3
7	6.763-11		4.287-	6	1.635-	5	3.033-	5	4.992-	5	1.593-	3

Table 79 THE FRANCIS FACTOR ACCORDING TO EAST 2)

	VV	V	1	2	3	4	5	
0	9.962-	4	2.659-	3	4.0116-	1	2.052-	5
1	2.766-	3	9.933-	1	3.0173-	3	2.531-	5
2	2.908-	4	3.0315-	3	9.911J-	1	2.573-	5
3	7.787-	3	1.976-	6	4.0609-	3	7.033-	6
4	1.075-	5	3.0150-	3	8.0459-	3	7.0224-	3
5	2.476-	5	6.661-	3	3.0313-	7	6.035-	1

Table 80 2K2 FRANCK-CONDON FACTORS = J2 (NO E - C)

$\nu\nu$	σ	1	2	3	4
0	3.963-1	2.212-3	5.820-4	2.265-4	4.373-9
1	2.233-3	9.959-1	2.103-4	2.084-4	3.983-4
2	5.353-4	5.357-4	9.371-1	1.169-4	1.373-4
3	2.374-4	2.291-4	1.309-4	9.339-1	2.533-3
4	8.161-6	4.040-4	2.211-4	3.175-3	9.785-1
5	1.239-5	1.003-5	0.096-4	6.496-4	1.454-2

Table 81

2K2 FRANCK-CONDON FACTORS: C22 (4C FEAST-HEATH)

γ	0	1	2	3	4	5	6	7								
0	3.955-	1	3.924-	3	1.002-	3	1.991-	3	1.058-	3	1.164-	6	1.342-	6	1.229-	6
1	3.941-	3	9.300-	1	4.633-	3	2.224-	4	1.553-	5	4.383-	7	1.021-	5	5.776-	9
2	1.449-	6	4.301-	3	9.999-	1	4.224-	3	5.245-	4	1.025-	6	1.061-	5	1.012-	7
3	1.297-	2	3.437-	4	3.155-	3	3.315-	4	5.006-	3	1.033-	4	1.304-	7	9.032-	5
4	7.116-	0	1.912-	6	8.360-	4	3.499-	3	3.912-	1	2.966-	3	1.309-	5	1.303-	0
5	3.460-	6	2.354-	7	3.128-	5	5.556-	4	2.697-	3	9.969-	1	2.334-	3	6.146-	4

Table 82

RK2 FRANCK-COMMON FACTORS FOR MO L - M

v	VV	0	1	2	3	4	5	6	7	8	9	10	11	
4	3.521-	3	2.233-	2	6.636-	2	1.362-	1	1.926-	1	1.656-	1	5.954-	2
4	1.586-	2	6.968-	2	1.333-	1	2.293-	1	5.536-	2	7.428-	4	3.381-	1
2	3.844-	2	1.114-	1	1.834-	1	2.602-	2	7.288-	3	7.434-	2	6.830-	2
3	6.636-	2	1.192-	1	1.125-	2	6.439-	3	6.617-	2	6.347-	4	3.166-	3
4	9.165-	2	8.955-	2	1.618-	3	6.807-	2	5.641-	2	3.639-	5	6.425-	2
5	1.869-	1	6.754-	2	1.111-	2	6.681-	2	7.644-	3	2.975-	2	5.195-	2
6	1.896-	1	1.469-	2	4.874-	2	3.987-	2	5.914-	3	5.326-	2	6.306-	3
7	1.006-	1	6.060-	4	5.778-	2	8.927-	3	3.401-	2	2.738-	2	6.089-	3

v	VV	12	13	14	15	16	17	18	19	20	21	22	23	
3	8.682-	4	1.724-	4	2.513-	5	6.710-	6	1.251-	6	3.497-	8	5.756-	9
2	1.839-	2	5.759-	3	1.459-	3	3.084-	4	5.756-	5	2.025-	5	6.394-	7
2	1.005-	1	5.206-	2	2.057-	2	6.563-	3	1.669-	3	3.398-	4	5.581-	5
3	1.212-	1	1.366-	1	9.768-	2	3.669-	2	1.931-	2	3.716-	3	1.351-	3
4	1.865-	4	5.059-	2	1.219-	1	1.337-	1	6.969-	2	4.281-	2	1.367-	2
5	7.457-	2	2.948-	2	2.221-	3	6.446-	2	1.260-	1	2.243-	1	7.006-	2
6	2.496-	4	6.132-	2	6.976-	2	1.586-	2	9.971-	3	6.382-	2	1.349-	1
7	6.686-	2	3.334-	2	1.188-	3	5.301-	2	5.929-	2	5.308-	3	2.465-	2

Table 83

RK2 FRANCK-CONDON FACTORS F(2) (3-2)

	VV	0	1	2	3	4	5	6	7	8	9	10	11
1	3.547-3	1.021-7	1.430-6	1.293-5	9.264-5	4.057-4	1.519-3	5.145-3	1.352-2	3.039-2	5.765-2	9.277-2	
2	3.449-6	9.091-7	1.142-5	9.071-2	5.105-4	2.107-3	7.154-3	1.075-2	3.910-2	6.537-2	8.637-2	8.593-2	
3	2.143-7	5.053-9	5.697-5	4.055-4	1.963-3	7.149-3	1.951-2	4.087-2	6.457-2	7.475-2	5.74-2	2.167-2	
4	9.135-7	1.951-5	1.979-4	1.231-3	5.243-3	1.011-2	3.523-2	5.909-2	3.621-2	4.494-2	1.050-2	1.697-3	
5	2.914-6	5.081-5	5.162-4	2.342-3	1.049-2	2.011-2	4.914-2	5.935-2	4.172-2	9.056-3	2.093-3	2.161-2	
6	7.663-6	1.361-4	1.113-3	5.419-3	1.726-2	3.713-2	5.255-2	4.372-2	1.330-2	4.503-4	2.222-2	3.347-2	
7	1.733-5	2.031-4	2.071-3	8.321-3	2.445-2	4.323-2	4.513-2	2.251-2	5.650-4	1.264-2	3.386-2	4.985-2	
8	3.498-2	5.191-4	3.426-3	1.317-2	3.092-2	4.420-2	3.326-2	6.545-3	3.409-3	2.297-2	2.552-2	2.222-3	
9	6.299-5	6.594-4	5.173-3	1.744-2	3.456-2	3.942-2	1.891-2	1.395-4	1.355-2	2.764-2	9.543-3	0.026-3	
10	1.013-4	1.269-3	6.936-3	2.074-2	3.527-2	3.0572-2	3.055-3	2.089-3	2.032-2	1.305-2	6.325-4	1.153-2	
11	1.477-4	1.724-3	6.606-3	2.292-2	3.306-2	2.145-2	1.590-3	7.520-3	2.137-2	8.797-3	1.391-3	1.793-2	
12	1.963-4	2.130-3	9.789-3	2.331-2	2.647-2	1.314-2	1.357-2	1.219-2	1.776-2	2.101-3	6.439-3	4.687-2	
13	2.399-4	2.449-3	1.036-2	2.225-2	2.307-2	7.126-3	3.339-4	1.417-2	1.190-2	2.467-5	1.445-2	2.161-2	
14	2.699-4	2.604-3	1.026-2	2.002-2	1.756-2	3.355-3	2.570-3	1.351-2	5.770-3	6.009-4	1.152-2	6.186-3	
15	2.817-4	2.561-3	9.579-3	1.711-2	1.299-2	1.333-3	3.913-3	1.155-2	3.330-3	2.051-3	1.027-2	2.572-3	
16	2.723-4	2.403-3	4.466-3	1.403-2	9.298-3	4.292-4	4.325-3	9.059-3	1.430-3	3.114-3	8.063-3	7.935-4	
17	2.461-4	2.113-3	7.151-3	1.112-2	6.523-3	9.298-5	4.214-3	6.749-3	5.230-4	3.323-3	5.902-3	4.417-4	
18	2.125-4	1.760-3	5.766-3	6.592-3	4.505-3	5.422-6	3.636-3	4.839-3	1.639-4	3.110-3	4.101-3	4.667-6	
19	1.736-4	1.414-3	6.495-3	6.412-3	3.111-3	3.486-6	3.029-3	3.610-3	3.630-5	2.043-3	2.793-3	2.395-5	
20	1.349-4	1.062-3	3.371-3	4.653-3	2.110-3	1.685-5	2.342-3	2.354-3	3.894-5	2.085-3	1.067-3	6.360-5	
21	8.605-5	6.991-4	2.147-3	2.903-3	1.253-3	2.134-3	1.519-3	1.410-3	3.432-8	1.367-3	1.090-3	6.390-5	

Table 83 (cont'd)

(3(2) 3-2)

v	v12	v13	v14	v15	v16	v17	v18	v19	v20	v21	v22	v23
1	1.275-1	1.50+1	1.519-1	1.32+1	9.974-2	6.595-2	3.823-2	1.936-2	6.476-3	3.236-3	1.131-3	3.809-4
1	5.850-2	1.973-2	1.965-5	1.946-2	6.821-2	1.143-1	1.311-1	1.153-1	8.112-2	2.381-2	1.090-2	
2	9.873-5	1.919-2	5.757-2	7.123-2	4.128-2	4.673-3	9.836-3	5.537-2	1.835-1	1.185-1	1.016-1	1.286-2
3	2.948-2	5.373-2	3.595-2	3.265-3	1.151-2	5.294-2	5.424-2	2.839-2	1.835-4	2.270-2	7.035-2	1.247-1
4	6.399-2	1.953-2	9.664-5	2.553-2	5.030-2	2.562-2	1.548-5	2.713-2	6.181-2	4.456-2	5.579-3	1.261-2
5	1.650-2	4.180-4	2.567-2	3.915-2	1.042-2	4.610-3	3.960-2	4.045-2	5.216-3	1.083-2	5.024-2	2.355-2
6	2.098-3	1.925-2	3.319-2	7.831-3	5.859-3	3.553-2	2.455-2	2.013-5	2.637-2	4.937-2	1.291-2	4.558-3
7	1.016-2	2.951-2	1.379-2	2.827-3	2.893-2	2.553-2	3.678-5	2.641-2	3.250-2	2.565-3	1.467-2	
8	2.289-2	1.683-2	2.783-5	2.006-2	2.179-2	1.946-4	1.937-2	2.695-2	1.271-3	1.093-2	3.355-2	2.264-3
9	2.132-2	2.657-3	6.799-3	2.279-2	3.439-3	9.299-3	2.434-2	3.387-3	1.111-2	2.883-2	5.036-3	1.004-2
10	1.125-2	9.031-4	1.753-2	1.120-2	1.162-3	2.045-2	3.271-3	3.071-3	2.396-2	8.444-3	4.573-3	2.337-2
11	2.768-3	0.113-3	1.647-2	1.611-3	9.465-3	1.049-2	1.035-4	1.433-2	1.432-2	2.637-4	1.696-2	1.171-2
12	1.355-5	2.085-2	9.787-3	3.250-4	1.375-2	6.591-3	2.036-3	1.642-2	2.546-3	8.232-3	1.716-2	3.825-4
13	1.061-3	2.161-2	3.783-3	3.265-3	1.222-2	9.211-4	9.039-3	1.040-2	1.833-4	1.378-2	6.924-3	2.689-3
14	2.952-3	9.543-3	7.701-4	5.631-3	7.936-3	6.335-3	3.935-3	4.173-3	3.015-3	1.200-2	8.901-4	7.743-3
15	6.119-3	0.039-3	7.226-6	6.552-3	4.254-3	1.103-3	9.537-3	9.595-4	5.446-3	7.475-3	1.145-4	9.114-3
16	6.315-3	6.361-3	1.850-4	5.920-3	1.939-3	2.160-3	3.191-3	4.037-5	5.990-3	3.763-3	1.220-3	7.697-3
17	3.866-3	2.647-3	4.926-4	4.713-3	7.722-4	2.555-3	4.056-3	9.117-5	5.216-3	1.610-3	2.126-3	5.319-3
18	3.106-3	1.584-3	6.641-4	3.517-3	2.737-4	2.414-3	2.549-3	2.938-4	4.058-3	6.205-4	2.371-3	3.425-3
19	2.424-3	3.462-4	5.741-4	2.502-3	9.452-5	2.013-3	1.532-3	4.135-4	2.942-3	2.130-4	2.142-3	2.212-3
20	1.555-3	2.023-4	5.107-4	2.0521-3	2.040-5	1.354-3	9.478-4	3.637-4	1.801-3	6.051-3	1.506-3	1.139-3

Table 84

RK2 FRANCK-CONDON FACTOR = C2 (V2 PHOTOL)

	W	U	1	2	3	4	5	6	7	8	9	10
3	9.039-1	9.274-2	3.310-3	6.414-3	4.072-7	6.058-3	8.334-12	7.0395-12	2.122-12	7.692-13	2.349-13	
4	8.956-2	7.291-1	1.714-1	9.792-3	1.697-6	2.366-3	4.187-6	6.936-11	7.605-11	2.051-11	7.548-12	
5	8.164-3	1.596-1	5.771-1	2.372-1	1.937-2	5.119-4	8.252-6	1.706-7	2.186-10	4.046-10	1.137-11	
6	3.635-4	1.709-2	2.439-1	4.654-1	2.910-1	3.212-2	1.110-3	2.241-3	5.340-7	5.525-11	1.565-9	
7	1.748-5	1.375-3	3.167-2	2.515-1	3.323-1	3.333-1	4.758-2	2.111-3	5.219-5	1.423-6	1.044-9	
8	5.822-7	8.796-5	3.294-3	4.998-2	2.758-1	2.366-1	3.542-1	6.630-2	3.679-3	1.095-4	3.393-6	
9	5.933-3	3.996-6	2.666-4	6.337-3	6.821-2	2.899-1	1.576-1	3.638-1	8.771-2	6.015-3	2.129-4	
10	2.942-11	9.195-6	1.586-5	6.356-4	1.070-2	8.656-2	2.917-1	9.492-2	3.921-1	1.117-1	9.367-3	
11	1.106-10	1.608-10	5.399-7	4.729-5	1.291-3	1.655-2	1.092-1	2.830-1	4.838-2	3.891-1	1.377-1	
12	3.046-13	3.240-10	3.199-9	2.591-6	1.197-4	2.347-3	2.460-2	1.232-1	2.649-1	1.767-2	3.750-4	
13	2.525-11	2.715-11	0.305-11	5.993-6	6.258-6	2.657-4	3.991-3	3.314-2	1.475-1	2.384-1	2.265-3	
14	2.965-11	2.695-10	4.348-11	1.737-3	4.092-7	2.390-5	5.372-4	5.354-3	4.392-2	1.629-1	4.352-1	
15	1.942-11	3.151-10	1.655-9	3.653-9	3.037-6	1.820-5	5.066-5	1.009-3	9.092-3	5.620-2	1.744-1	
16	1.047-11	2.239-10	1.603-9	7.545-9	2.098-6	2.065-7	6.317-6	1.399-4	1.784-3	1.417-2	6.964-2	
17	4.762-12	1.268-11	1.455-9	6.109-9	2.033-6	3.458-6	9.217-7	1.646-5	2.925-4	2.995-3	1.996-2	
18	2.242-12	6.710-11	0.625-10	6.302-9	2.908-6	9.337-6	3.538-7	3.245-5	4.750-5	5.745-4	4.910-3	
19	1.145-12	3.358-11	4.828-10	4.102-9	2.332-6	9.045-9	2.825-7	1.153-6	9.704-5	1.105-4	1.003-3	
20	5.712-13	1.680-11	2.612-10	2.492-9	1.618-8	7.329-9	2.513-7	7.645-7	3.396-6	2.565-5	2.366-4	
21	2.989-13	0.692-12	1.414-11	1.438-9	1.020-8	5.273-8	2.922-7	6.474-7	2.037-5	9.020-6	6.147-5	
22	1.531-13	4.762-12	7.827-11	6.226-9	3.519-6	1.325-7	5.247-7	1.565-6	4.995-6	2.208-5	1.155-4	
23	7.727-14	2.779-12	4.466-11	4.799-10	3.759-9	2.258-9	1.862-7	3.993-7	1.247-6	3.591-6	1.155-5	

Table 84 (cont'd)

(V2 PHOT 1)

v	VV	11	12	13	14	15	16	17	18	19	20
0	5.287-14	1.278-14	1.015-14	1.016-14	1.017-14	1.018-14	1.019-14	1.020-14	1.022-14	1.024-14	
1	2.502-12	3.373-13	3.463-13	1.151-13	3.938-14	1.040-14	1.154-14	1.021-14	1.023-14	1.025-14	
2	4.285-11	1.593-11	5.812-12	2.207-12	6.977-13	3.958-13	1.879-13	9.036-14	3.062-14	1.025-14	
3	4.533-10	1.791-10	7.068-11	2.789-11	1.121-11	4.958-12	2.198-12	9.691-13	4.061-13	1.546-13	
4	4.895-9	1.455-9	6.068-10	2.537-10	1.066-10	4.377-11	1.995-11	8.720-12	3.762-12	1.535-12	
5	4.269-9	1.327-8	4.090-9	1.770-9	7.733-10	3.372-10	1.481-10	6.573-11	2.955-11	1.161-11	
6	7.464-9	5.620-9	3.221-8	1.013-8	4.533-9	2.054-9	2.45-10	4.116-10	1.016-10	7.867-11	
7	3.946-4	1.244-5	1.213-11	7.136-8	2.270-8	1.047-8	1.938-9	2.231-9	1.046-9	4.353-11	
8	4.442-2	6.941-4	3.038-5	3.111-9	1.468-7	6.660-8	2.268-9	1.036-8	4.785-9	2.153-9	
9	1.653-1	2.032-2	1.153-3	5.736-5	2.855-5	2.839-7	6.795-9	4.252-8	2.015-9	9.274-9	
10	3.545-1	1.934-1	2.060-2	1.882-3	1.046-4	1.330-4	1.194-7	1.545-7	7.593-8	3.573-8	
11	1.235-3	3.164-1	2.210-1	3.925-2	2.956-3	1.851-4	4.539-7	9.041-7	2.525-7	1.249-7	
12	1.672-1	1.363-2	2.744-1	2.466-1	5.259-2	4.622-3	3.197-4	1.370-6	1.505-6	3.053-7	
13	1.866-1	1.269-1	3.537-2	2.265-1	2.682-1	3.859-2	6.992-3	5.331-4	3.598-6	2.386-6	
14	8.366-2	1.813-1	6.729-2	6.513-2	1.757-1	2.951-1	6.828-2	1.035-2	6.773-4	6.536-6	
15	2.721-2	9.745-2	1.729-1	5.175-2	9.643-2	1.254-1	2.343-1	1.136-1	1.351-1	1.402-3	
16	7.416-3	3.531-2	1.099-1	1.580-1	2.356-2	1.316-1	7.929-2	2.98-1	1.356-1	2.130-2	
17	4.065-3	1.191-2	4.591-2	1.196-1	1.302-1	5.521-3	1.577-1	4.123-2	2.853-1	1.624-1	
18	4.724-4	3.113-3	1.577-2	5.682-2	1.252-1	1.059-1	1.747-1	1.457-2	2.663-1		
19	1.357-4	6.959-4	4.996-3	2.191-2	5.796-2	1.258-1	7.851-2	7.214-3	1.785-1	1.444-3	
20	5.329-5	2.783-4	1.575-3	7.633-3	2.903-2	7.829-2	1.196-1	4.876-2	2.593-2	1.673-1	

Table 85

2K2 FRANCK-CONDON FACTOR : J2 (V2 P401) 21

v	vv	u	1	2	3	4	5	6	7	8	9	10	
1	2.726-	1	3.027-	1	8.499-	2	2.000-	2	3.265-	3	3.845-	4	
1	3.137-	1	2.549-	2	1.126-	1	2.712-	1	1.870-	1	1.509-	2	
2	2.155-	1	2.454-	2	1.577-	1	7.501-	5	1.593-	1	2.354-	1	
3	1.116-	1	1.584-	1	9.216-	3	1.346-	1	5.250-	2	4.216-	2	
4	4.953-	2	1.598-	1	3.709-	2	8.140-	2	4.159-	2	1.198-	1	
5	2.011-	2	1.084-	1	1.112-	1	8.667-	4	1.139-	1	3.672-	5	
6	7.625-	3	5.959-	2	1.237-	1	3.437-	2	3.950-	2	1.658-	2	
7	2.838-	3	2.898-	2	9.442-	2	8.842-	2	3.244-	4	8.133-	2	
8	1.015-	3	1.293-	2	5.845-	2	1.015-	1	3.493-	2	1.697-	2	
9	3.641-	4	5.513-	3	3.163-	2	8.146-	2	7.451-	2	2.724-	3	
10	1.	1.315-	4	2.280-	3	1.596-	2	5.443-	2	8.429-	2	3.472-	2
11	4.713-	5	9.270-	4	7.581-	3	3.221-	2	7.063-	2	6.474-	2	
12	1.719-	5	3.736-	4	3.478-	3	1.753-	2	5.000-	2	7.223-	2	
13	6.283-	5	1.591-	4	1.561-	3	9.098-	3	3.155-	2	3.226-	2	
14	2.342-	5	6.639-	5	6.912-	4	4.539-	3	1.645-	2	6.532-	2	
15	8.821-	7	2.440-	5	3.030-	4	2.210-	3	1.024-	2	3.053-	2	
16	3.385-	7	9.920-	5	1.331-	4	1.059-	3	5.479-	3	1.091-	2	
17	1.315-	7	4.063-	6	2.826-	5	2.021-	4	2.659-	3	1.114-	2	
18	5.046-	8	1.676-	6	2.555-	5	2.306-	4	1.466-	3	6.335-	3	
19	1.942-	8	6.949-	7	1.123-	5	1.111-	4	7.424-	4	3.511-	3	
20	7.435-	9	2.686-	7	4.952-	5	5.205-	5	3.729-	4	1.910-	3	

Table 85 (cont'd)

(N2 PHOTC 2)

v	VV	11	12	13	14	15	16	17	18	19	20
1	2.543-14	5.037-12	4.259-12	5.291-12	4.372-14	3.254-13	3.745-13	4.152-14	4.027-14	9.086-14	
2	3.881-8	1.659-9	6.307-12	6.779-12	2.336-11	3.578-13	5.044-12	2.353-12	7.549-14	8.626-13	
3	5.306-6	2.432-7	6.292-9	1.162-11	1.026-14	3.074-11	5.110-12	3.372-12	6.258-12	4.703-13	
4	6.901-3	8.495-4	7.003-6	3.664-6	3.480-19	3.631-12	3.983-11	1.019-11	3.251-12	4.093-11	
5	6.272-2	1.422-2	2.049-3	1.941-4	2.233-5	3.214-7	1.131-9	2.357-10	4.709-11	2.242-11	
6	1.909-1	9.501-2	2.642-2	4.380-3	6.754-4	3.396-5	1.586-5	4.156-6	8.148-10	6.189-11	
7	9.519-2	1.956-1	1.296-1	4.311-2	8.483-3	1.053-3	8.47-5	4.374-6	1.317-7	2.584-9	
8	3.359-2	3.971-2	1.826-1	1.515-1	3.562-2	1.512-2	2.144-3	1.931-4	1.106-5	3.703-7	
9	6.412-2	7.333-2	6.165-3	1.456-1	1.641-1	3.259-2	2.516-2	4.051-3	4.104-4	2.584-5	
10	5.440-2	2.293-2	9.925-2	1.714-2	9.751-2	1.323-1	1.219-1	3.834-2	7.219-3	8.161-4	
11	3.782-3	7.728-2	1.110-3	9.896-2	2.214-2	5.017-2	1.934-1	1.511-1	5.746-2	1.211-2	
12	6.353-2	3.258-3	7.392-2	6.722-3	7.453-2	5.452-2	1.515-2	1.579-1	1.736-1	7.924-2	
13	4.243-2	3.294-2	2.491-2	4.873-2	3.165-2	3.935-2	8.34-2	3.377-4	1.206-1	1.835-1	
14	1.587-3	5.593-2	7.491-3	5.020-2	1.867-2	5.873-2	1.058-2	9.617-2	6.694-3	7.894-2	
15	1.473-2	1.770-2	5.025-2	3.402-4	3.159-2	1.244-3	1.131-2	1.958-7	8.86-2	2.843-2	
16	4.234-2	7.312-4	3.037-2	2.855-2	1.311-2	3.24-2	4.49-3	6.474-2	9.828-3	6.348-2	
17	4.209-2	2.291-2	4.500-3	4.798-2	7.366-3	3.44-2	2.972-2	2.335-2	4.217-2	3.254-2	
18	2.116-2	4.112-2	5.266-3	2.076-2	4.036-2	7.736-5	4.895-2	8.125-3	4.486-2	1.678-2	
19	3.593-3	3.473-2	2.734-2	2.375-4	3.654-2	2.152-2	9.526-3	4.733-2	9.538-6	5.566-2	
20	6.358-4	1.539-2	3.778-2	1.015-2	3.334-3	4.353-2	4.739-3	2.732-2	3.088-2	8.415-3	

Table 86

KK2 FRANCK-CONDON FACTOR = J2 (V2 PHOTO 3)

V	VV	0	1	2	3	4	5	6	7	8	9	10
4	6.843- 1	1.627- 1	1.150- 2	1.279- 3	1.595- 4	2.364- 5	4.335- 6	9.339- 7	2.685- 7	9.332- 6	2.927- 6	
5	1.131- 1	6.656- 1	1.567- 1	2.943- 2	4.316- 3	7.237- 4	1.323- 5	2.831- 5	7.336- 5	2.297- 6	7.668- 7	
6	2.579- 3	2.653- 1	2.296- 1	2.052- 1	4.969- 2	9.873- 3	1.377- 3	4.333- 4	1.098- 4	3.240- 3	1.092- 5	
7	3.851- 7	6.563- 3	2.612- 1	4.901- 1	2.134- 1	6.995- 2	1.716- 2	4.139- 3	1.071- 3	3.110- 4	1.026- 4	
8	2.516- 5	1.260- 5	1.093- 2	3.448- 1	3.171- 1	2.030- 1	6.752- 2	2.535- 2	7.439- 3	2.215- 3	7.263- 4	
9	3.210- 9	1.440- 5	9.047- 3	1.479- 2	3.992- 1	2.481- 1	1.829- 1	1.412- 1	3.513- 2	1.195- 2	4.030- 3	
0	1.796- 9	3.202- 14	4.746- 5	3.720- 4	7.39- 2	4.469- 1	4.974- 1	1.543- 1	2.134- 1	4.403- 2	5.728- 2	
1	4.214- 11	2.466- 8	7.227- 6	1.134- 4	1.138- 3	1.813- 2	4.894- 1	1.613- 1	2.208- 1	1.150- 1	5.148- 2	
2	3.532- 14	3.446- 11	1.536- 7	1.132- 6	2.182- 4	2.864- 3	1.553- 2	5.258- 1	2.365- 1	8.556- 2	2.155- 1	
3	6.700- 12	1.173- 11	6.336- 10	6.295- 7	7.476- 6	3.425- 4	3.282- 3	1.295- 2	5.579- 1	1.207- 1	5.266- 2	
4	1.506- 12	5.711- 11	6.754- 11	2.033- 6	1.840- 6	3.322- 5	4.256- 4	1.237- 2	7.434- 3	5.798- 1	2.118- 1	
5	1.028- 14	3.343- 11	2.775- 10	3.382- 10	1.903- 7	3.869- 5	1.144- 4	3.755- 4	2.221- 2	2.091- 3	5.873- 4	
6	1.029- 14	6.572- 12	2.240- 10	4.009- 10	4.156- 10	1.093- 5	5.321- 6	3.245- 4	1.488- 4	3.659- 4	2.936- 5	
7	1.743- 13	6.510- 13	2.959- 11	7.595- 10	9.030- 11	8.239- 11	4.373- 6	2.842- 5	7.796- 4	1.826- 5	5.522- 5	
8	2.044- 13	1.062- 14	3.069- 14	1.023- 10	1.569- 9	2.146- 9	5.672- 6	1.475- 5	1.140- 6	1.566- 3	1.147- 3	
9	1.030- 14	4.422- 13	4.180- 12	5.251- 12	2.835- 10	3.796- 13	3.246- 8	7.055- 7	3.676- 5	6.039- 5	2.690- 3	
10	1.490- 13	6.323- 13	4.337- 12	3.725- 11	5.631- 11	4.646- 11	2.235- 9	1.542- 7	5.912- 5	5.659- 5	4.264- 4	
11	2.698- 13	3.321- 13	2.178- 12	2.988- 11	2.421- 10	2.531- 11	1.343- 10	8.362- 9	3.095- 7	2.492- 5	7.018- 5	
12	7.414- 14	3.720- 14	5.689- 13	1.183- 11	1.633- 10	1.800- 9	5.833- 10	6.153- 9	6.778- 7	6.750- 6	9.133- 5	
13	1.348- 14	1.691- 14	2.405- 14	1.912- 12	4.337- 11	6.322- 10	2.424- 9	6.166- 10	1.972- 7	2.928- 6	2.864- 6	
14	1.280- 13	6.246- 14	5.241- 14	2.545- 14	1.626- 12	1.216- 10	3.746- 9	2.140- 9	6.521- 10	1.079- 6	6.645- 6	

Table 86 (cont'd)

(N2 PHOTC 3)

V	VV	11	12	13	14	15	16	17	18	19	20	
1	1.0 J24-	8	3.0 835-	9	1.0 524-	9	5.0 885-10	2.0 210-10	9.0 131-11	1.0 533-11	6.0 857-12	5.0 148-12
1	2.0 912-	7	1.0 131-	7	4.0 525-	8	1.0 852-	8	7.0 739-	9	3.0 322-	9
2	4.0 066-	6	1.0 620-	6	6.0 740-	7	2.0 895-	7	1.0 209-	7	5.0 555-	8
3	3.0 792-	5	1.0 225-	5	6.0 534-	6	2.0 900-	6	1.0 329-	6	3.0 132-	7
4	2.0 664-	4	1.0 173-	4	4.0 653-	5	2.0 127-	5	1.0 077-	5	4.0 855-	5
5	1.0 487-	3	5.0 985-	4	2.0 613-	4	1.0 215-	4	3.0 910-	5	2.0 972-	3
6	6.0 537-	3	2.0 725-	3	1.0 241-	3	5.0 632-	4	2.0 815-	4	1.0 456-	4
7	2.0 343-	2	1.0 090-	2	4.0 582-	3	2.0 196-	3	1.0 114-	3	5.0 925-	4
8	5.0 337-	2	2.0 332-	2	3.0 417-	2	7.0 129-	3	3.0 713-	3	2.0 316-	3
9	1.0 126-	1	5.0 767-	2	3.0 589-	2	1.0 864-	2	5.0 811-	3	3.0 386-	3
10	2.0 386-	2	1.0 078-	1	5.0 459-	2	4.0 106-	2	2.0 292-	2	1.0 439-	2
11	1.0 079-	1	2.0 144-	3	1.0 325-	1	4.0 576-	2	4.0 437-	2	2.0 520-	2
12	5.0 732-	1	1.0 568-	1	3.0 826-	4	9.0 812-	2	3.0 429-	2	4.0 715-	2
13	6.0 562-	3	5.0 297-	1	4.0 352-	1	1.0 374-	2	9.0 617-	2	2.0 754-	2
14	7.0 547-	2	2.0 793-	2	4.0 510-	1	9.0 655-	2	4.0 693-	2	3.0 753-	2
15	6.0 441-	3	9.0 136-	2	6.0 858-	2	3.0 398-	1	6.0 174-	2	3.0 554-	2
16	3.0 538-	3	2.0 113-	2	9.0 406-	2	1.0 265-	1	2.0 382-	1	2.0 251-	2
17	1.0 754-	3	3.0 035-	3	5.0 145-	2	7.0 591-	2	1.0 840-	1	9.0 314-	2
18	9.0 952-	0	5.0 152-	3	9.0 835-	4	9.0 970-	2	3.0 951-	2	2.0 112-	1
19	2.0 394-	4	1.0 779-	4	1.0 118-	2	9.0 323-	4	1.0 434-	1	3.0 932-	3
20	4.0 325-	5	3.0 814-	4	2.0 325-	3	1.0 678-	2	1.0 716-	2	1.0 646-	1
									4.0 511-	3	7.0 925-	2
									2.0 375-	2	6.0 831-	2

Table 87

KKR FRANCK-CONDON FACTOR = J2 (42 PHOT) 4)

V	W	J	1	2	3	4	5	6	7	8	9	10
1	2.797-	3	2.213-	2	1.911-	2	1.643-	1	2.365-	1	1.557-	1
2	1.413-	2	7.391-	2	1.504-	1	1.352-	1	3.248-	2	1.024-	2
3	3.731-	2	1.222-	1	1.171-	1	1.051-	2	3.177-	2	1.077-	1
4	6.852-	2	1.293-	1	3.508-	2	1.172-	2	6.762-	2	1.957-	2
5	9.834-	2	3.339-	2	1.955-	7	6.936-	2	3.161-	2	1.749-	2
6	1.145-	1	4.331-	2	2.397-	2	6.227-	2	9.055-	4	0.316-	2
7	1.243-	1	6.603-	3	5.913-	2	1.889-	2	3.400-	2	5.255-	2
8	1.172-	1	3.616-	4	6.547-	2	3.520-	5	5.456-	2	2.955-	4
9	1.017-	1	1.182-	2	4.643-	2	1.595-	2	3.360-	2	1.792-	2
10	2.54-	2	3.654-	2	2.355-	2	3.398-	2	6.297-	3	0.099-	2
11	6.319-	2	4.592-	2	3.765-	3	4.039-	2	9.670-	4	3.636-	2

V	W	11	12	13	14	15	16	17	18	19	20	
0	2.708-	5	4.217-	6	4.536-	5	1.073-11	7.0.431-11	2.322-11	1.533-11	2.134-14	
1	2.770-	3	1.410-	4	1.533-	7	2.834-	7	2.082-11	3.511-	2.370-10	
2	4.541-	2	7.356-	3	4.241-	4	3.416-	7	9.126-	7	3.347-	9
3	1.865-	1	6.169-	2	1.575-	2	9.747-	4	5.979-	7	2.086-	5
4	1.213-	1	2.139-	1	1.226-	1	2.793-	2	1.086-	5	6.379-	8
5	1.436-	2	6.185-	2	2.154-	1	1.640-	1	4.414-	2	3.405-	3
6	5.836-	2	4.731-	2	1.945-	2	1.945-	1	2.022-	1	5.496-	2
7	2.933-	2	2.256-	2	7.283-	2	5.491-	4	1.575-	1	2.334-	1
8	8.232-	3	5.112-	2	2.782-	3	7.737-	2	6.045-	3	1.129-	1
9	4.431-	2	6.670-	4	5.041-	2	3.770-	3	5.224-	2	6.796-	2
10	1.561-	2	2.396-	2	1.536-	2	3.375-	2	2.121-	2	3.518-	2

Table 88

TABLE 88 FRANCE-COMMON FACTORS (1940-1942)

v	v	0	1	2	3	4	5	6	7	8	9	10	11							
1	2.297-	1	2.953-	1	2.227-	1	1.311-	1	6.695-	2	3.113-	2	3.591-	3	2.317-	3	3.626-	4	3.622-	4
2	3.899-	1	4.771-	2	2.491-	2	4.188-	1	1.468-	1	1.158-	1	7.426-	2	4.128-	2	2.109-	2	4.015-	2
3	2.666-	1	9.472-	2	1.639-	1	2.223-	2	1.398-	2	7.513-	2	1.365-	1	3.531-	2	6.859-	2	4.256-	3
4	3.398-	2	2.967-	1	5.630-	5	1.184-	1	9.006-	2	7.041-	3	1.459-	2	3.012-	2	9.439-	2	6.070-	2
5	1.880-	2	2.048-	1	1.914-	1	4.962-	2	3.537-	2	1.036-	1	4.667-	2	6.514-	4	1.739-	2	5.259-	2
6	1.774-	3	5.637-	2	2.674-	1	7.630-	2	1.094-	1	4.112-	4	6.813-	2	7.474-	2	2.112-	2	2.262-	4
7	7.537-	5	7.384-	3	1.144-	2	2.745-	1	1.251-	2	1.251-	1	1.435-	2	2.524-	2	7.217-	2	4.682-	2
8	2.105-	6	3.811-	4	1.022-	2	1.676-	1	2.468-	1	9.958-	4	1.015-	1	4.572-	2	2.162-	3	4.066-	2
9	2.102-	9	4.639-	5	1.097-	3	3.661-	2	2.187-	1	1.937-	1	2.161-	2	5.234-	2	7.153-	2	3.965-	3
10	6.526-	9	1.413-	3	1.153-	5	2.322-	3	3.214-	2	2.593-	1	1.359-	1	5.334-	2	2.717-	2	7.055-	2
11	8.433-11		2.745-	6	1.652-	7	2.139-	5	4.095-	3	7.945-	2	2.073-	1	6.690-	2	8.125-	2	6.076-	3
12	6.774-10		1.971-	3	1.237-	4	8.590-	7	2.927-	5	6.397-	3	1.061-	1	7.032-	1	6.530-	2	9.792-	2
13	3.307-10		6.721-	3	2.933-11		3.057-	6	2.565-	6	3.356-	5	3.120-	3	1.339-	1	3.091-	1	2.062-	2
14	3.529-11		6.271-11		1.032-	6	2.636-	9	3.908-	6	6.226-	6	2.846-	5	1.221-	2	1.658-	1	3.084-	1
			4.698-11		1.504-	9	5.315-	9	1.195-	6	4.734-	8	1.418-	5	1.124-	5	1.457-	2	3.047-	1

Table 88 (cont'd)

(C(2) C(3))

V	V	12	13	14	15	16	17	18	19	20	21	22	23
Y	Y	2.0595- 3	2.0219- 2	3.0308- 6	3.0532- 6	1.0377- 6	5.0159- 7	1.0856- 7	5.0515- 8	2.0424- 3	1.0113- 3	7.0123- 3	5.036- 3
1	2	9.166- 4	3.0356- 4	2.0077- 4	7.0122- 5	3.030- 5	2.0239- 5	5.0239- 5	2.0625- 6	1.0457- 6	5.0122- 6	2.0517- 7	1.0332- 7
2	3	0.397- 3	3.106- 3	1.0471- 3	3.052- 4	3.101- 4	1.0528- 4	3.0776- 4	3.0191- 5	1.0531- 5	7.0527- 0	3.0765- 3	1.0930- 6
3	4	2.036- 2	1.0378- 2	7.0037- 3	3.0879- 3	1.0975- 3	9.0225- 4	4.0959- 4	2.0494- 4	1.0249- 4	6.0376- 3	3.0299- 5	1.075- 3
5	6	5.320- 2	3.0699- 2	2.0349- 2	1.0406- 2	6.056- 3	4.0460- 3	2.0462- 3	1.0462- 3	7.036- 4	3.0771- 4	2.0421- 4	1.073- 4
7	8	0.069- 2	5.0761- 2	4.0065- 2	3.0336- 2	2.0216- 2	1.0336- 2	8.0454- 3	4.0950- 3	2.087/- 3	1.0643- 3	9.0279- 4	5.0130- 4
9	10	2.0290- 2	4.0353- 2	3.0270- 2	4.0990- 2	4.0075- 2	3.0417- 2	2.0465- 2	1.0375- 2	9.0714- 3	5.0393- 3	3.0229- 3	1.0916- 3
11	12	1.0422- 3	5.026- 3	2.0418- 2	4.0504- 2	4.0606- 2	4.0333- 2	3.000- 2	2.0739- 2	1.0958- 2	2.0421- 3	3.0421- 3	5.0501- 3
13	14	4.0144- 2	1.0199- 2	3.0346- 7	8.0500- 3	2.0434- 2	3.0225- 2	4.0438- 2	3.0798- 2	3.0197- 2	2.0694- 2	3.0629- 2	1.0257- 2
15	16	3.046- 2	4.0747- 2	2.0581- 2	4.0379- 3	7.0379- 4	3.0451- 2	2.0353- 2	3.0254- 2	3.0542- 2	3.0339- 2	2.0636- 2	2.0196- 2
17	18	1.0167- 4	2.0116- 2	4.0236- 2	3.0596- 2	1.0466- 2	1.0223- 3	2.0336- 3	1.0153- 2	2.0205- 2	2.0897- 2	3.0094- 2	2.0029- 2
19	20	2.0037- 2	0.0191- 3	3.0412- 3	3.0149- 2	3.0199- 2	2.0432- 2	7.0688- 3	1.0212- 4	3.0213- 3	1.0172- 2	2.0099- 2	2.0451- 2
21	22	3.0136- 2	5.0467- 2	1.0751- 2	3.0192- 4	1.0616- 2	3.0474- 2	3.0474- 2	1.0467- 2	3.0800- 3	3.0154- 5	3.0927- 3	1.071- 2
23	24	1.0692- 2	1.0496- 2	3.0192- 2	2.0687- 2	1.0549- 3	7.0307- 3	2.0604- 2	2.0262- 2	2.0412- 2	1.0073- 2	2.0776- 3	2.0330- 4
25	26	3.0204- 2	3.0115- 2	4.0353- 3	6.0123- 2	3.0632- 2	7.0616- 3	1.0202- 3	1.0535- 2	2.0033- 2	2.001- 2	1.001- 2	6.059- 3

Table 89

RK2 FRANCK-CONDON FACTORS FOR (C2) PAIR 21

VV	0	1	2	3	4	5	6	7	8	9	10	11
V	3.041- 3	5.379- 2	1.372- 1	2.139- 1	2.286- 1	1.789- 1	1.059- 1	6.837- 2	1.726- 2	6.986- 3	1.121- 3	2.034- 4
0	3.586- 2	1.226- 1	1.575- 1	7.425- 2	7.369- 4	5.057- 2	1.493- 1	1.794- 1	1.303- 1	6.637- 2	2.546- 2	7.129- 3
1	7.159- 2	1.406- 1	3.138- 2	1.966- 3	8.123- 2	9.044- 2	3.478- 2	2.111- 2	1.183- 1	1.567- 1	1.292- 1	6.234- 2
2	1.040- 1	1.023- 1	1.517- 3	6.166- 2	7.033- 2	4.483- 4	5.897- 2	6.917- 2	2.045- 2	2.192- 2	2.193- 1	1.637- 1
3	1.234- 1	4.672- 2	1.672- 2	7.731- 2	3.973- 3	6.885- 2	5.326- 2	7.685- 2	6.313- 2	7.641- 2	5.298- 3	3.923- 2
4	1.272- 1	9.153- 3	5.664- 2	3.237- 2	1.681- 2	6.155- 2	3.328- 2	5.626- 2	6.189- 2	4.117- 2	7.623- 2	5.676- 2
5	1.182- 1	3.226- 4	6.650- 2	1.131- 3	5.464- 2	1.324- 2	3.262- 2	4.301- 2	3.797- 3	6.484- 2	1.775- 2	2.254- 2
6	1.016- 1	1.237- 2	5.120- 2	3.040- 3	4.778- 2	3.158- 3	3.247- 2	4.120- 2	5.086- 2	1.760- 2	2.341- 2	5.544- 2
7	6.226- 2	3.205- 2	2.434- 2	3.460- 2	1.671- 2	3.031- 2	2.372- 2	2.202- 2	3.376- 2	6.263- 2	5.148- 2	3.735- 2
8	6.357- 2	4.922- 2	5.269- 3	4.621- 2	2.240- 4	4.669- 2	2.380- 3	4.394- 2	7.707- 4	4.333- 2	7.014- 3	3.072- 2
9	4.726- 2	5.698- 2	6.006- 5	4.316- 2	7.522- 3	3.033- 2	1.339- 2	2.575- 2	1.644- 2	2.969- 2	1.625- 2	3.791- 2
10												

VV	12	13	14	15	16	17	18	19	20	21	22	23
V	2.909- 3	2.815- 0	1.937- 7	3.215- 6	7.362- 9	9.432- 10	1.727- 9	1.376- 9	5.689- 10	1.529- 9	7.663- 13	9.381- 14
0	1.563- 3	2.571- 4	3.139- 5	3.459- 6	3.256- 7	2.915- 9	2.822- 9	2.856- 9	3.359- 9	1.781- 10	1.980- 9	
1	2.378- 2	3.347- 3	1.203- 3	3.037- 4	2.045- 5	1.635- 6	7.655- 6	4.280- 6	1.356- 9	3.722- 10	5.214- 10	9.373- 10
2	1.165- 1	5.492- 2	1.601- 2	6.228- 3	7.204- 4	9.058- 5	8.406- 6	6.641- 7	1.054- 9	1.408- 9	3.247- 11	1.129- 10
3	1.350- 4	1.532- 1	3.660- 2	3.944- 2	1.112- 2	2.014- 3	3.135- 4	3.834- 5	1.909- 6	9.752- 6	2.276- 6	5.065- 3
4	6.553- 5	7.062- 2	1.524- 1	1.363- 1	7.109- 2	2.618- 2	5.591- 3	8.931- 4	9.951- 5	8.241- 6	7.942- 7	1.728- 7
5	9.310- 2	2.493- 2	1.351- 2	1.121- 1	1.576- 1	1.892- 1	4.487- 2	1.215- 2	2.243- 3	2.986- 3	3.374- 5	4.050- 5
6	7.211- 4	5.420- 2	6.841- 2	1.064- 3	5.392- 2	1.458- 1	1.617- 1	7.296- 2	2.368- 2	5.121- 3	8.491- 4	1.230- 4
7	5.091- 2	3.064- 2	1.032- 2	3.186- 2	7.873- 2	1.186- 2	9.955- 3	1.110- 1	1.530- 1	4.101- 2	1.049- 2	2.334- 3
8	2.771- 2	1.215- 2	3.686- 2	2.787- 3	4.789- 2	6.651- 2	1.577- 3	5.896- 2	1.342- 1	6.632- 2	2.242- 2	
9	2.636- 3	4.937- 2	1.836- 3	4.515- 2	3.132- 2	1.816- 2	7.839- 2	2.694- 2	1.530- 2	1.542- 1	1.024- 1	
10												

Table 90

TABLE 90
FRANCK-COOPSON FACTORS FOR CLOUET

VV	0	1	2	3	4	5	6	7	8	9	10	11
V	$2.925 - 3$	$1.975 - 2$	$5.361 - 2$	$1.290 - 1$	$1.851 - 1$	$2.937 - 1$	$1.705 - 1$	$1.154 - 1$	$6.472 - 1$	$3.003 - 2$	$1.161 - 2$	$3.919 - 3$
1	$1.303 - 2$	$3.123 - 2$	$1.243 - 1$	$1.397 - 1$	$6.295 - 2$	$3.826 - 3$	$2.641 - 2$	$9.970 - 2$	$1.500 - 1$	$4.333 - 1$	$9.92 - 2$	$5.327 - 2$
2	$3.137 - 2$	$3.941 - 2$	$1.119 - 1$	$3.594 - 1$	$2.525 - 3$	$6.251 - 2$	$9.192 - 2$	$3.716 - 2$	$1.633 - 1$	$1.162 - 1$	$1.416 - 1$	$1.162 - 1$
3	$5.474 - 2$	$1.135 - 1$	$5.250 - 2$	$5.501 - 2$	$5.664 - 2$	$6.598 - 2$	$6.142 - 3$	$2.427 - 2$	$6.005 - 2$	$5.427 - 2$	$2.503 - 3$	$2.634 - 2$
4	$7.762 - 2$	$9.156 - 2$	$7.387 - 3$	$3.253 - 2$	$9.314 - 2$	$5.819 - 3$	$2.767 - 2$	$5.691 - 2$	$1.695 - 2$	$1.212 - 2$	$6.901 - 2$	$5.794 - 2$
5	$9.507 - 2$	$5.691 - 2$	$2.617 - 3$	$5.912 - 2$	$2.311 - 2$	$1.328 - 2$	$2.625 - 2$	$1.848 - 2$	$1.869 - 2$	$2.987 - 2$	$1.672 - 2$	$9.655 - 3$
6	$1.464 - 1$	$2.417 - 2$	$2.396 - 2$	$6.824 - 2$	$4.043 - 3$	$4.322 - 2$	$2.078 - 2$	$1.336 - 2$	$5.009 - 2$	$9.557 - 3$	$1.649 - 2$	$5.613 - 2$
7	$1.052 - 1$	$4.439 - 3$	$4.531 - 2$	$1.966 - 2$	$1.662 - 2$	$3.959 - 2$	$1.353 - 4$	$6.161 - 2$	$1.682 - 2$	$1.216 - 2$	$6.680 - 2$	$5.051 - 3$
8	$9.910 - 2$	$2.710 - 4$	$5.131 - 2$	$1.526 - 3$	$3.708 - 2$	$1.222 - 2$	$1.804 - 2$	$3.133 - 2$	$1.519 - 3$	$4.049 - 2$	$9.206 - 3$	$1.710 - 2$
9	$6.410 - 2$	$7.758 - 3$	$4.243 - 2$	$3.191 - 3$	$3.831 - 2$	$3.666 - 6$	$3.645 - 2$	$4.851 - 3$	$4.469 - 2$	$2.187 - 2$	$5.796 - 3$	$3.456 - 2$
10	$7.469 - 2$	$2.354 - 2$	$2.546 - 2$	$1.667 - 2$	$2.278 - 2$	$9.357 - 3$	$2.737 - 2$	$2.536 - 3$	$3.292 - 2$	$4.126 - 4$	$3.015 - 2$	$1.456 - 2$
VV	12	13	14	15	16	17	18	19	20	21	22	23
V	$1.092 - 3$	$2.549 - 1$	$5.432 - 5$	$9.441 - 6$	$1.509 - 6$	$1.243 - 7$	$6.726 - 9$	$7.036 - 9$	$2.887 - 9$	$2.596 - 9$	$2.578 - 11$	$2.045 - 3$
1	$2.265 - 2$	$6.327 - 3$	$2.332 - 3$	$5.673 - 4$	$1.156 - 4$	$1.919 - 5$	$2.628 - 6$	$3.612 - 7$	$6.279 - 8$	$2.616 - 10$	$3.031 - 10$	$2.490 - 9$
2	$1.118 - 1$	$6.519 - 2$	$2.934 - 2$	$1.052 - 2$	$3.074 - 3$	$7.421 - 4$	$1.473 - 4$	$2.357 - 5$	$3.137 - 6$	$3.932 - 7$	$5.429 - 9$	$1.232 - 9$
3	$3.919 - 2$	$1.304 - 1$	$1.143 - 1$	$6.862 - 2$	$3.124 - 2$	$1.116 - 2$	$3.195 - 3$	$7.362 - 4$	$1.384 - 4$	$2.295 - 5$	$3.949 - 6$	$7.153 - 7$
4	$6.796 - 3$	$2.116 - 2$	$9.233 - 2$	$1.329 - 1$	$1.128 - 1$	$6.592 - 2$	$2.967 - 2$	$1.821 - 2$	$2.807 - 3$	$6.413 - 4$	$1.347 - 4$	$2.633 - 5$
5	$6.552 - 2$	$5.524 - 2$	$3.942 - 3$	$2.313 - 2$	$9.532 - 2$	$1.316 - 1$	$1.473 - 1$	$5.386 - 2$	$2.569 - 2$	$6.634 - 3$	$2.404 - 3$	$6.243 - 4$
6	$1.346 - 2$	$1.229 - 2$	$5.598 - 2$	$6.866 - 2$	$1.509 - 3$	$3.972 - 2$	$1.428 - 1$	$1.231 - 1$	$9.003 - 2$	$5.264 - 2$	$2.229 - 2$	$6.151 - 3$
7	$2.290 - 2$	$5.233 - 2$	$7.69 - 3$	$1.873 - 2$	$6.759 - 2$	$3.678 - 2$	$6.842 - 7$	$6.256 - 2$	$1.897 - 1$	$1.220 - 1$	$6.051 - 2$	$4.992 - 2$
8	$4.191 - 2$	$1.565 - 3$	$3.155 - 2$	$4.629 - 2$	$2.294 - 3$	$2.921 - 2$	$6.034 - 2$	$2.679 - 2$	$1.789 - 3$	$5.458 - 2$	$1.140 - 1$	$1.251 - 1$
9	$3.042 - 3$	$2.579 - 2$	$3.429 - 2$	$4.362 - 3$	$3.944 - 2$	$3.654 - 2$	$4.065 - 5$	$6.241 - 2$	$6.444 - 2$	$1.542 - 2$	$7.407 - 3$	$7.727 - 2$
10	$1.338 - 2$	$3.323 - 2$	$2.796 - 3$	$3.602 - 2$	$2.352 - 2$	$3.535 - 3$	$6.675 - 2$	$2.433 - 2$	$3.211 - 3$	$5.232 - 2$	$5.355 - 2$	$4.391 - 3$

Table 91
RK2 FRANCK-CONDON FACTORS FOR C(2) C(2) C(2) C(2)

	VV	0	1	2	3	4	5	6	7	8	9	10	11
V	4.120-1	3.731-1	1.612-1	4.376-2	8.425-3	3.246-3	1.568-4	1.436-5	9.136-5	6.006-6	9.964-9	5.366-14	
1	3.373-1	2.065-3	2.316-1	2.605-1	1.233-1	3.236-2	7.304-3	1.126-3	1.335-3	1.219-5	1.162-5	1.179-7	
2	1.620-1	1.714-1	8.146-2	4.739-2	2.284-1	1.359-1	8.476-2	2.344-2	6.664-3	7.057-4	8.514-2	9.396-6	
3	6.059-2	2.117-1	1.790-1	1.611-1	2.692-3	1.157-1	1.458-1	1.426-1	1.383-2	1.387-2	2.687-3	3.991-9	
4	1.973-2	1.364-1	1.324-1	1.509-2	1.186-1	6.439-2	2.149-2	1.696-1	1.836-1	9.734-2	3.284-2	7.959-3	
5	5.936-3	6.476-2	1.597-1	3.306-2	8.252-2	3.213-2	1.206-1	2.232-3	8.342-2	1.846-2	1.432-1	6.333-2	
6	1.708-3	2.616-2	1.117-1	1.141-1	4.962-4	1.339-1	6.189-4	1.053-1	6.974-2	1.496-2	1.363-1	1.712-1	
7	4.770-4	9.442-3	9.032-2	1.265-1	4.241-2	3.629-2	5.927-2	3.573-2	4.332-2	9.795-2	3.644-3	6.379-2	
8	1.296-4	3.192-3	2.739-2	3.443-2	2.034-1	1.437-3	7.067-3	1.392-2	6.193-2	1.605-3	9.504-2	4.151-2	
9	3.332-5	1.014-3	1.420-2	5.479-2	1.063-1	4.239-2	1.453-2	7.541-2	2.839-3	7.830-2	1.631-2	4.742-2	
10	7.705-6	3.022-4	4.237-3	2.732-2	8.206-2	8.737-2	5.020-3	5.230-2	3.283-2	3.767-2	3.269-2	5.694-2	
	VV	12	13	14	15	16	17	18	19	20	21	22	23
V	1.726-10	2.077-12	3.963-11	6.649-11	1.025-11	2.536-11	9.725-11	1.796-11	2.619-11	6.013-11	9.083-12	7.437-12	
1	3.482-9	2.626-11	1.032-10	2.521-10	1.263-10	9.332-11	5.221-11	6.070-11	7.163-11	1.166-10	9.734-12	1.930-13	
2	6.076-7	9.367-9	1.139-11	3.936-9	1.612-9	1.122-9	5.946-10	1.111-9	1.185-11	9.693-11	3.038-11	2.041-6	
3	4.717-5	3.934-6	1.765-6	4.386-6	1.631-6	3.033-9	2.588-9	2.357-9	6.609-10	1.916-9	3.34-11	1.443-9	
4	1.403-3	1.936-4	2.121-5	1.893-6	1.987-7	6.010-9	2.343-9	1.312-9	2.492-9	2.089-9	3.127-10	1.453-9	
5	1.902-2	4.168-3	6.976-4	9.111-5	9.025-6	8.037-7	5.461-5	1.119-9	5.998-11	1.298-9	7.753-10		
6	1.027-1	3.937-2	1.057-2	2.137-3	3.240-4	3.894-5	4.099-5	2.898-7	7.683-7	1.677-9	1.205-11		
7	1.646-1	1.611-1	6.981-2	2.316-2	5.586-3	1.027-3	1.446-4	1.689-5	1.316-6	1.103-7	3.442-8	1.205-9	
8	1.123-2	1.193-1	1.014-1	1.066-1	4.464-2	1.309-2	2.051-3	6.695-4	6.322-5	7.330-6	1.172-6	3.110-7	
9	6.461-2	3.323-3	2.530-2	1.493-1	1.433-1	7.543-2	2.712-2	7.893-3	1.612-3	2.622-4	4.145-5	8.924-6	
10	4.514-3	8.621-2	3.947-2	7.800-3	1.035-1	1.366-1	1.112-1	5.026-2	1.623-2	4.074-3	9.277-4	2.192-4	

Table 92

442 FRANCK-COJONON FACTORS FOR (002) PHOTON

<i>VV</i>	<i>0</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>5</i>	<i>6</i>	<i>7</i>	<i>8</i>	<i>9</i>	<i>10</i>	<i>11</i>
<i>v</i>	6.750- -1	1.538- -1	2.110- -1	2.679- -1	1.619- -1							
1	1.943- -1	1.621- -1	2.627- -2	1.542- -2	1.268- -2	9.076- -2	6.091- -2	1.278- -2	1.136- -1	1.136- -1	1.136- -1	1.136- -1
2	2.538- -1	4.170- -2	1.268- -2	1.268- -2	4.064- -2	4.064- -2	1.122- -3	5.323- -2	7.045- -2	5.278- -2	5.278- -2	5.278- -2
3	2.299- -1	3.952- -1	9.644- -2	9.644- -2	2.323- -2	2.323- -2	2.092- -3	6.699- -2	6.246- -2	6.148- -2	6.148- -2	6.148- -2
4	1.522- -1	9.628- -2	3.323- -2	3.323- -2	1.796- -1	1.796- -1	5.131- -2	3.956- -2	4.174- -3	3.962- -2	3.873- -2	3.873- -2
5	7.592- -2	1.796- -1	7.360- -1	7.360- -1	2.777- -2	1.734- -1	5.121- -2	2.692- -4	5.053- -2	2.692- -4	5.272- -3	5.197- -2
6	7	6.589- -3	1.140- -4	1.419- -4	8.433- -4	3.896- -2	3.411- -2	7.045- -2	6.555- -2	1.524- -2	9.663- -3	4.645- -2
7	6.293- -4	4.733- -2	1.639- -1	3.533- -2	2.958- -2	3.762- -2	5.113- -2	1.059- -2	1.155- -2	6.520- -2	6.925- -3	1.375- -2
8	5.144- -5	1.222- -2	1.222- -2	1.169- -1	1.229- -1	7.753- -4	1.753- -2	3.293- -2	1.077- -2	3.524- -2	2.069- -3	2.102- -2
9	1.0	3.981- -4	9.251- -4	5.933- -2	1.577- -1	2.699- -2	1.946- -2	6.511- -4	6.750- -2	5.891- -3	4.391- -2	3.546- -2

<i>VV</i>	<i>12</i>	<i>13</i>	<i>14</i>	<i>15</i>	<i>16</i>	<i>17</i>	<i>18</i>	<i>19</i>	<i>20</i>	<i>21</i>	<i>22</i>	<i>23</i>
<i>v</i>	8.760- -5	1.869- -5	3.0744- -0	7.019- -0	1.427- -7	1.427- -7	1.427- -7	1.427- -7	1.427- -7	1.427- -7	1.427- -7	1.427- -7
1	2.903- -3	6.643- -4	2.251- -4	2.367- -5	1.125- -5	1.755- -6	2.393- -7	5.301- -6	9.783- -9	7.302- -11	1.122- -11	6.998- -13
2	2.836- -2	1.162- -2	4.136- -2	3.424- -3	1.260- -3	7.619- -5	4.532- -5	2.774- -6	6.429- -7	6.119- -8	2.226- -9	6.137- -9
3	9.726- -2	6.246- -2	3.249- -2	1.362- -2	4.087- -3	1.591- -3	3.933- -4	8.787- -5	1.682- -5	3.023- -6	5.340- -7	1.190- -7
4	9.477- -2	1.116- -1	9.712- -2	3.332- -2	1.430- -2	1.430- -2	1.968- -3	1.676- -3	3.738- -3	6.689- -5	1.002- -5	4.231- -6
5	1.105- -4	2.701- -2	6.149- -2	1.683- -1	3.473- -2	6.177- -2	3.146- -2	1.334- -2	6.434- -3	1.339- -3	3.639- -4	9.451- -5
6	6.148- -2	2.842- -2	3.537- -2	2.893- -2	8.252- -2	1.877- -1	9.095- -2	3.717- -2	2.825- -2	1.147- -2	4.596- -3	1.379- -3
7	6.516- -4	3.740- -2	5.466- -2	2.311- -2	2.996- -4	3.435- -2	6.673- -2	1.056- -1	8.453- -2	5.113- -2	2.545- -2	1.136- -2
8	4.729- -2	1.827- -2	2.666- -3	4.210- -2	5.449- -2	2.658- -2	2.033- -3	6.207- -2	8.985- -2	7.368- -2	5.0475- -2	2.036- -2
9	2.587- -3	2.926- -2	6.396- -2	1.101- -2	6.503- -3	4.765- -2	6.937- -2	1.931- -2	5.522- -3	4.936- -2	9.236- -2	1.031- -2
10	2.596- -2	3.006- -2	9.333- -3	2.666- -2	4.015- -2	5.291- -2	1.291- -2	6.224- -2	6.934- -3	1.006- -2	6.204- -2	6.204- -2

Table 93
2x2 FRANCK-COURN FACTORS FOR C(12) IN C(2)

v	11	10	9	8	7	6	5	4	3	2	1	v
0	3.722	1	1.212	1	2.933	6	1.554	3	3.397	5	2.556	6
1	3.049	2	1.623	1	2.249	1	1.642	3	2.042	4	1.655	9
2	3.234	2	1.356	1	3.146	1	1.482	2	5.918	3	5.717	3
3	3.708	4	7.724	2	1.479	1	3.297	1	3.692	1	2.446	2
4	3.295	4	3.754	3	1.329	1	1.396	1	2.129	2	2.923	2
5	2.337	6	1.703	3	7.774	3	1.933	1	2.304	2	2.321	2
6	7.696	0	6.564	7	5.171	5	1.279	2	2.447	1	1.272	1
7	5.316	6	6.124	2	1.542	3	1.031	2	1.816	2	1.95	2
8	3.715	6	2.476	2	2.340	4	6.517	5	1.966	2	2.451	2
9	1.227	5	1.614	2	9.712	5	6.542	4	3.143	2	3.120	1
10	2.754	7	3.048	3	6.329	5	2.355	4	1.447	3	2.951	2
11												3.676
12												1.094
13												2.530
14												1.306
15												1.743
16												5.678
17												5.303
18												2.192
19												7.246
20												3.122
21												1.647
22												2.493
23												4.039

Table 94

TABLE OF FRANCK-CONDON FACTORS BY VARIOUS INVESTIGATORS

<u>Molecule</u>	<u>System</u>	<u>Reference</u>
CN	Red (A-X)	33
CN	Violet (B-X)	33
CO	4(+) (A-X)	33
CO ⁺	Comet tail (A-X)	34
CO ⁺	(1-) (B-X)	34
N ₂	(1+) (B-A)	33, 35, 36, 37, 29
N ₂	(2+) (C-B)	33, 35, 36, 37
N ₂	Vegard Kaylan (A-X)	35, 37, 29
N ₂	y bands (B'-B)	36
N ₂	y bands (a-a')	36
N ₂	y bands (w-a)	36
N ₂	LBH (a-x)	37
N ₂	Tanaka (c-x)	37
N ₂	B-H (b', b-x)	33
N ₂ ⁺	Meinel (A-X)	33
N ₂ ⁺	(1-) (B-X)	33
N ₂ ⁺	(2-) (C-X)	33
NO	β (A-X)	33, 38
NO	γ (B-X)	33, 38
NO	δ (C-X)	33
NO	ϵ (D-X)	33
NO	β' (B'-X)	33
NO	γ' (E-X)	33

Table 94 (cont'd)

<u>Molecule</u>	<u>System</u>	<u>Reference</u>
NO	Lagerquist-Miescher (G-X)	33
NO	Heath (C-A)	
NO	Feast 1 (D-A)	33
NO	Feast 2 (E-A)	33
	Feast 2 (E-C)	33
NO	Feast-Heath (E-D)	33
O ₂	Schumann-Runge (B-X)	33, 39

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APPENDIX I

COMPUTER PROGRAM TURNGPT

A listing of the computer program used to generate the RK potentials at AFWL is included in this appendix. The input data needed is described and a sample data deck is also included.

1. INPUT DATA

The reduced mass of the molecule or the mass at each atom is needed. These can be based on either C₁₂ or O₁₆. A good source for reduced masses based on O₁₆ is Herzberg (Ref. 31).

The energy levels of the molecule can be constructed internally in the program if the spectroscopic constants we, wexe, weye, weze, wete are read in. These are used in the equation.

$$\begin{aligned} E = & \text{we}(v+\frac{1}{2}) - \text{wexe}(v+\frac{1}{2})^2 + \text{weye}(v+\frac{1}{2})^3 \\ & + \text{weze}(v+\frac{1}{2})^4 + \text{wete}(v+\frac{1}{2})^5 + \dots \end{aligned}$$

Herzberg (Ref. 31) has a large tabulation of these. Alternatively, one can use the G_v obtained from spectroscopic data. Wallace (Refs. 24, 40) has an extensive tabulation of these.

One also needs the relational constants, that is, either B_e, α_e, δ_e, γ_e, ε_e, or the B_v for the various vibrational levels. Again Herzberg (Ref. 31) is a good source for B_e, α_e, γ_e and Wallace (Refs. 24, 40) is a good source for the B_v. The final bit of data about the molecule that is needed is the equilibrium internuclear separation. This can be found in Herzberg (Ref. 31).

2. DATA DECK

The data deck set-up procedure needs very little explanation since Zare has made extensive use of comment cards throughout his program.

Card Number

1	I TEST I1	1 if problem follows
2, 3	FMT 8A10	Title of the problem with carriage control in column 1
4	IIMS, ZMAS1, ZMAS2 IF, 2E10.0	IIMS = 1 mass based on C = 12 IIMS = 2 mass based on O = 16 ZMAS1 mass of first atom (or reduced mass of molecule) ZMAS2 mass of second atom (or blank when using reduced mass)
5	IQHK, N 2I4, 4x, 6A10	IQHK = 0 using a tabulated Gv curve. Format for Gv in columns 13-72. IQHK ≠ 0 using constants to generate Gv curve. Hollerith text in columns 13-72.
		N - number of vibrational levels to be used
6a	WE, WEXE, WEYE, WEZE, WETE, 5E10.0	Use when IQHK ≠ 0. These are the spectroscopic constants that generate the energies of the vibrational levels.
6b	G(I) Format in columns 13-72 of Card 5	Use when IQHK = 0. These are the Gv of spectroscopy.
7	IOPEV I1	IOPEV = 0 if zero point energy to be found by extrapolation IOPEV = 1 tabulated Gv curve to be used unchanged IOPEV = 2 if Gv curve is to be constructed from constants
8	IBHK, N 2I4, 4x	IBHK = 0 using tabulated Bv curve. Format for Bv in columns 13-72.

Card Number

Card 8 (cont'd)

		IBHK ≠ 0 constants are used to generate Bv curve. Hollerith text in columns 13-72.
		N - number at vibrational levels (same as above)
9a	BE, ALPHAE, GAMMAE, DELTAE, 5E10.0	Use when IBHK ≠ 0; these were used to generate the Bv
9b	B(v) Format in columns 13-72 of Card 8	Use when IBHK = 0 •
10	IOPA, BEQUIL I4, 3F10.0	IOPA = 0 value of BE to be found by extrapolation from Bv data read in IOPA = 1 value of BE given by BEQUIL IOPA = 2 rotational constants are used (leave BEQUIL blank)
		BEQUIL - spectroscopic constant Be
11	RE F10.0	Internuclear equilibrium distance
12	VSTART, VFIN, HDED 3E10.0	Turning points are calculated from vibrational level VSTART to VFIN to steps of HDED
13	IOPFG I1	IOPFG = 0 intermediate printout skipped IOPFG = 1 intermediate steps in an evaluation of the Klein integrals are to be printed out
14	Blank	

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PROGRAM TURNORT(INPUT,OUTPUT,TAPES=INPUT,TAPE6=OUTPUT,FILMPL,PUNCH A 1
1,TAPE7=PUNCH) A 2
C   SET-UP FOR PLOTTING POTENTIALS... A 3
C   CALL INIT2RC A 4
C   MAIN FINDS TURNING POINTS FOR A MOLECULE BY RYDBERG-KLEIN-OPFS. NET A 5
C   ALL INPUT IS IN WAVE NUMBERS AND ANGSTROMS. A 6
C   USER SPECIFIES CHOICE BETWEEN MASS UNITS BASED ON C12 = 12, OR A 7
C   O16 = 16. A 8
C   THE FOLLOWING COMMENT CARDS DESCRIBE THE PREPARATION OF DATA CARDS A 9
C
C
C   DIMENSION VSTART(1), VFIN(1), HDER(1) A 10
C   DIMENSION XI(200), YI(200), X0(200), Y(200), SV(200), F A 11
C   ITIAL(200), QIPAI(2), QIFN(3), QIMS(2), ZIMS(2), ZIPAI(2), ZIFN(2), A 12
C   ZFCALC(200), XPRN(5), VPRN(5), DTERMT(6), G(200), PV(200), FMT(16), A 13
C   Z(U(200)), PMIN(200), PMAX(200), DUFM(16), PVF(200), GI(200), RV(20 A 14
C   40), J(20), PV(30), PVF(30), PVE1(30), PVE2(30), A(30), Y(30), XX(6 A 15
C   5), YY(6), ANS(3), XNN(5), XFL(1), XFE(1), FL(1), DB(30), YY A 16
C   6Y(6), SIGH(1) A 17
C   COMMON XI,YI,X0,Y,XH,NSTA,N,NSTA,M,XMIN,XMAX,INSC,MREG,NUSED,S,N1, A 18
C   INS,MAXIT,FACM,ZMU,DE,WE,WEXF,WFYF,WZEF,WTF,PF,ALPHAF,GAMMAF,DELTA A 19
C   2F,AS,BS,NO,STEP,U,PV,G,ICK,H,ITR,HDES,PSLNF,XY,REQUIL,ZPTFN,MLV,L A 20
C   ?V,RF,VSTART,VFIN,HDER A 21
C   REAL J1,J2,J3,J4,JHAF2 A 22
C
C   FIRST CARD IN DATA HAS A ONE IN COLUMN 1 IF A PROBLEM FOLLOWS. A 23
C   VERY LAST CARD IN DATA MUST BE A BLANK CARD..... A 24
C
C   CONTINUE A 25
C   READ (5,50) ITEST A 26
C   IF (ITEST) 2,60,2 A 27
C
C   NEXT TWO CARDS IN DATA HAVE NAME OF PROBLEM IN COLUMNS 1-60. A 28
C   WHERE CARRIAGE CONTROL IS IN COLUMN 1. NEXT CARD HAS IIMS AND A 29
C   MASSES OF THE TWO ATOMS, OR IIMS AND REDUCED MASS IN FIRST MASS A 30
C   FIELD WITH SECOND BLANK. A 31
C   IIMS = 1, MASS UNITS ARE BASED ON C12 = 12. A 32
C   IIMS = 2, MASS UNITS ARE BASED ON O16 = 16. A 33
C
C   READ (5,51) (ENTL(I),I=1,16) A 34
C   READ (5,52) ITMS,ZMAS1,ZMAS2 A 35
C
C   NEXT CARD IN DATA HAS IQHK, AND NUMBER OF LEVELS, EACH A 36
C   IN 14 FORMAT, AS WELL AS THE FORMAT STATEMENT WHICH CONTROLS THE A 37
C   READING OF THE LEVELS (IN COLUMNS 12-72)--FOR EXAMPLE- (4F16.8). A 38
C   IQHK = 0 IF THE FOLLOWING CARDS CONTAIN THE TABULATED G CURVE. A 39
C   IF A PARTICULAR VALUE IS TO BE INTERPOLATED, SET G(1) = -10. A 40
C   IF IT IS DESIRED TO USE CONSTANTS TO GENERATE THE ENTIRE A 41
C   G CURVE, IQHK MUST NOT BE EQUAL TO ZERO. A 42
C   A FOLLERITH TEXT MUST BE PUNCHED IN COLUMNS 12-72. A 43
C   AS IT WILL BE PRINTED, E.G., (1H ) A 44
C   THE NEXT CARD IN SUCH A CASE CONTAINS A 45
C   WE,WEXF,WFYF,WZEF,AND WTF. A 46
C
C   READ (5,53) IQHK,N,(DTERMT(I),I=1,6) A 47
C   ITME2 A 48
A 49
A 50
A 51
A 52
A 53
A 54
A 55

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3 IF (IQHK) 3,4,2 A 56
READ (5,54) WF,WEXF,WEYF,WEZF,WETF A 57
GO TO 5 A 58
4 READ (5,DTFRMT) (GI(I),I=1,N) A 59
C A 60
C THE ZERO POINT ENERGY MAY BE FOUND BY EXTRAPOLATION, OR IT MAY BE A 61
C FIXED BY THE USER FROM HIS TABULATED G(V) CURVE. A 62
C NEXT CARD CONTAINS IOPEV. A 63
C SET IOPEV = 0, IF THE ZERO POINT ENERGY IS TO BE FOUND BY A 64
C EXTRAPOLATION, AND THE G(V) CURVE IS TO BE RAISED OR LOWERED A 65
C ACCORDINGLY. A 66
C THIS IS PARTICULARLY USEFUL IF DELTA G(V) DATA IS TO BE USED. A 67
C SET IOPEV = 1, IF THE TABULATED G(V) CURVE IS TO BE USED UNCHANGED A 68
C SET IOPEV = 2, IF THE G(V) CURVE IS TO BE CONSTRUCTED FROM CONSTAN A 69
C A 70
5 READ (5,50) IOPEV A 71
C A 72
C THE NEXT SET OF CARDS CONTAINS THE PV CURVE WITH THE SAME A 73
C RESTRICTIONS AS FOR G CURVE ABOVE. NUMBER OF VALUES HERE MUST BE A 74
C EQUAL TO THE NUMBER ABOVE A 75
C A 76
C READ (5,53) TBHK,N,(DUENT(I),I=1,6) A 77
C IIFB=2 A 78
C IF (IBHK) 6,7,6 A 79
6 READ (5,54) BF,ALPHAF,GAMMAF,DELTAf,EPSLNF A 80
C GO TO 8 A 81
7 READ (5,DUENT) (RV(I),I=1,N) A 82
C A 83
C THE ROTATIONAL CONSTANT BF MAY BE FOUND BY EXTRAPOLATION, OR IT A 84
C MAY BE FIXED BY THE USER. A 85
C NEXT CARD CONTAINS IOPA AND REQUIL. A 86
C SET IOPA = 0, IF THE VALUE OF BE IS TO BE FOUND BY EXTRAPOLATION A 87
C FROM THE RV DATA READ IN. LEAVE REQUIL BLANK. A 88
C SET IOPA = 1, IF THE VALUE OF BE IS TO BE GIVEN BY REQUIL. A 89
C SET IOPA = 2, IF ROTATIONAL CONSTANTS ARE USED. LEAVE REQUIL A 90
C BLANK. A 91
C A 92
8 READ (5,52) IOPA,REQUIL A 93
C A 94
C READ IN HIGHER TERMS IN EXPANSION HV,HV,COUPLING CONSTANT A,LAMDA, A 95
C GAMMA OF A MULLIKEN FORMULA,NUMBER OF J LEVELS TO BE CALCULATED NJ, A 96
C AND IND (=1 2 3) TO INDICATE EXPANSION FORM 1 FOR SINGLET SIGMA A 97
C 2 FOR DOUBLET PI 1/2 3 FOR DOUBLET PI 3/2 A 98
C IND=5 F1 DOUBLET SIGMA A 99
C IND=6 F2 DOUBLET SIGMA A 100
C A 101
C READ (5,55) HV,LAM,NJ,GAM,IND A 102
C READ (5,56) (DV(I),I=1,N) A 103
C READ F6, (A(I),I=1,N) A 104
C A 105
C READ ROTATIONAL LEVELS J A 106
C A 107
C READ (5,57) (J(I),I=1,NJ) A 108
C A 109
C NEXT DATA CARD CONTAINS RE, THE INTERNUCLEAR EQUILIRIUM DISTANCE. A 110

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```

C READ (5,5F) VF
C
C NEXT DATA CARD CONTAINS VSTART, VFIN, AND HDIF WHERE
C TURNING POINTS ARE CALCULATED FROM VIBRATIONAL LEVEL VSTART TO
C VFIN IN STEPS OF HDIF. F.G. FROM 0.5 TO 20.5 IN STEPS OF 1.0.
C
C READ (5,5F) VSTART,VFIN,HDIF
C
C NEXT CARD CONTAINS IOREG.
C SET IOREG = 1, IF INTERMEDIATE STEPS IN THE EVALUATION OF THE
C KLEIN ACTION INTEGRALS ARE TO BE PRINTED.
C SET IOREG = 0, IF INTERMEDIATE PRINT-OUT IS TO BE SKIPPED.
C NORMALLY THE USER SHOULD SET IOREG = 0.
C
C READ (5,5F) IOREG
C READ 60, 02
C READ 61, (02(I),I=1,2)
C THIS TERMINATES COMMENT CARDS ON THE PREPARATION OF DATA.
C IF NO FURTHER PROBLEMS FOLLOW, REMEMBER TO ADD A BLANK CARD TO
C THE DATA DECK.
C
C QIRAI(2)=6HANGST.
C QIFN(2)=6H1/C"
C QIMS(1)=6HC12=12
C QIMS(2)=6H016=16
C
C PRINT HEADING
C
C WRITE (6,5I) (FMT(1),I=1,16)
C WRITE (6,5I) (FMT(1),I=1,16)
C
C PRINT THE MASSES AND THEIR UNITS.
C
C IF (ZMAS2) 10,10,0
C WRITE (6,6I) QIMS(1)IMS, ZMAS1,ZMAS2
C GO TO 11
C WRITE (6,6I) QIMS(1)IMS, ZMAS1
C
C PRINT G(V) DATA, OR VIBRATIONAL CONSTANTS
C
C 11 IF (10HK) 12,12,12
C 12 WRITE (6,DTERM1)
C 13 WRITE (6,64) WF,WEXF,WEXE,WEXZ,WETE
C 14 GO TO 14
C 15 WRITE (6,6F) QIFN(1)FN
C 16 WRITE (6,6I) (01(I),I=1,4)
C 17 WRITE (6,6T)
C
C PRINT DV DATA, OR ROTATIONAL CONSTANTS
C
C 18 IF (10HK) 15,15,15
C 19 WRITE (6,DTERM1)

```

```

      WRITE (6,68) RF,ALPHAE,GAMMAE,DELTAE,ERSLNE
      GO TO 17
16   WRITE (6,69) OIFN1(IFB)
      WRITE (6,70) (RVI(I),I=1,N)
      WRITE (6,67)

C      PRINT HEADING
17   WRITE (6,51) (FMT(I),I=1+16)
C
      IF (ZMAS2) 18,19,19
18   ZMU=ZMAS1
      GO TO 20
19   ZMU=ZMAS1*ZMAS2/(ZMAS1+ZMAS2)
20   ZIMS(1)=1.0
      ZIMS(2)=.9996794
      ZIRA(1)=1.0
      ZIRA(2)=1.889765
      ZMU=ZMU*ZIMS(1)MS1
      ZIFN(1)=ZMU*3.64366F2
      ZIFN(2)=ZMU*1.6610826F-2
      ZIFN(3)=ZMU*1.339776F2
      FACM=60.201702/ZMU
      XI(1)=0.5
      DO 21 I=2,N
      IL=I-1
      YI(I)=YI(IL)+1.0
21   CONTINUE
      ZERO=0.0
C      CALCULATE THE BV TO BE USED IN LATER COMPUTATION OF POTENTIALS
C
      J1=0.
      DO 49 LJ=1,NJ
      J4=J(LJ)
      LAM2=LAM*LAM
C      IND=4 FOR TRIPLET SIGMA STATE
      GO TO (22,24,26,28,35,27,30,39), IND
C      SINGLET SIGMA ELECTRONIC STATES
C
22   J2=J4*(J4+1)
      DO 23 I=1,N
      PV(I)=RVI(I)-2.*PV(I)*J2+HV*J2*J2
      PVF=PV(I)*J2-PV(I)*J2*J2+HV*J2*J2*J2
      G(I)=G(I)+PVF
      GR(I)=G(I)
23   CONTINUE
      GO TO 41
C      DOUBLET PI 1/2 ELECTRONIC STATE - HILL AND VAN VLECK-
C
C      F1
24   J4AF2=(J4+.5)*F2.
      J2=2*J4+1
      J1=J4+(-1)**(IND+1)**.5

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```

DO 26 I=1,N                                         A 220
R=RV(I)(I)SA1=A(I)SY1=A1/RSD=DV(I)             A 221
RV(I)=R*(1.-(4.*JHAF2+Y1)*(Y1-4.)*LAM2)**-.5)-1./J3*(4.*D*J4**3.-.5*16AM)
RVE=R*(JHAF2-LAM2-.5*(4.*JHAF2+Y1)*(Y1-4.)*LAM2)**.5)-D*J4**4.+.5*G   A 222
18M*(J4-.5)                                         A 223
G(I)=GI(I)+RVE                                     A 224
GR(I)=G(I)                                         A 225
CONTINUE                                           A 226
GO TO 41                                         A 227
A 228
A 229
A 230
A 231
A 232
A 233
A 234
A 235
A 236
A 237
A 238
A 239
A 240
A 241
A 242
A 243
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A 262
A 263
A 264
A 265
A 266
A 267
A 268
A 269
A 270
A 271
A 272
A 273
A 274

25
C DOUBLET PI 3/2 ELECTRONIC STATE - HILL AND VAN VLECK-          A 231
C
C F2
26
JHAF2=(J4+.5)**2.
J1=J4+(-1)**(IND+1)*.5
J3=2*J4+
DO 27 I=1,N
R=RV(I)(I)SA1=A(I)SY1=A1/RSD=DV(I)
RV(I)=R*(1.+(4.*JHAF2+Y1)*(Y1-4.)*LAM2)**-.5)-1./J3*(4.*D*J4**3.+.5*16AM)
RVE=R*(JHAF2-LAM2+.5*(4.*JHAF2+Y1)*(Y1-4.)*LAM2)**.5)-D*(J4+1.)*4.-.5*GAM*(J4+.5)
G(I)=GI(I)+RVE
GR(I)=G(I)
CONTINUE
GO TO 41
A 232
A 233
A 234
A 235
A 236
A 237
A 238
A 239
A 240
A 241
A 242
A 243
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A 245
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A 247
A 248
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A 271
A 272
A 273
A 274

27
C TRIPLET SIGMA ELECTRONIC STATE
C
C A-IS COUPLING PARAMETER LAMBDA,A IS EMPTY FOR THIS CALCULATION
C J(PROGRAM)=K(PHYSICAL)
C IFP=1 --- F1 ,IFP=2 --- F2 ,IFP=3 -- F3
28
IFP=2
DO TO (20,31,33), IFP
C
F1
29
J3=2*J4+
J2=J4*(J4+1)
DO 30 I=1,N
R=RV(I)(I)SA1=A(I)SD=DV(I)
J4R=(2*J4+3)*R
TSQ=J4R**J4R-A1*A1-2*A1*R
TSQ=AMAY1(0.,TSQ)
TSQ=TSQ**.5
RV(I)=R-2*D*J2+1./J3*(2*R-2*J4R*R/TSQ+GAM)
RVE=R+J2-D*J2*J2+J4R-A1-TSQ+GAM*(J4+1)
G(I)=GI(I)+RVE
GR(I)=G(I)
CONTINUE
GO TO 41
A 250
A 251
A 252
A 253
A 254
A 255
A 256
A 257
A 258
A 259
A 260
A 261
A 262
A 263
A 264
A 265
A 266
A 267
A 268
A 269
A 270
A 271
A 272
A 273
A 274

30
F2
31
J2=J4*(J4+1)
DO 32 I=1,N
R=RV(I)(I)SA1=A(I)SD=DV(I)
RV(I)=R-2*D*J2
A 270
A 271
A 272
A 273
A 274

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      RVE=R*J2-D*J2*J2          A 275
      G(I)=G(I)+RVE            A 276
      GB(I)=G(I)                A 277
32    CONTINUE                 A 278
      GO TO 41                  A 279
C     F3
33    J2=J4*(J4+1)             A 280
      J3=2*J4+1                A 281
      DO 34 I=1,N               A 282
      R=RV(I) S C=A(I) SD=DV(I) A 283
      J4R=(2*J4-1)*R           A 284
      TSQ=J4R*J4R+A1*A1-2*A1*R A 285
      TSQ=AMAX1(0.,TSQ)        A 286
      TSQ=(TSQ)**.5            A 287
      RV(I)=R-2*D*J2+1/J3*(-2*R+2*J4R*R/TSQ-GAM) A 288
      RVE=R*J2-J4R-A1+TSQ-GAM*J4-D*J2*J2          A 289
      G(I)=G(I)+RVE            A 290
      GB(I)=G(I)                A 291
34    CONTINUE                 A 292
      GO TO 41                  A 293
C
C     DOUBLET SIGMA ELECTRONIC STATE
C
C     A=GAM FOR THIS CALCULATION
C     J IS ACTUALLY K SINCE WE HAVE CASE B COUPLING
C     F1
35    J3=2*J4+1                A 294
      J2=J4*(J4+1)             A 295
      J1=J4                      A 296
      DO 36 I=1,N               A 297
      R=RV(I) S C=A(I) SD=DV(I) A 298
      RV(I)=R*(1.-2.*D*J2/R-C/(2.*J3*R))          A 299
      RVE=R*J2-D*J2*J2-C*J2/2.                      A 300
      G(I)=G(I)+RVE            A 301
      GB(I)=G(I)                A 302
36    CONTINUE                 A 303
      GO TO 41                  A 304
C     F2
37    J3=2*J4+1                A 305
      J2=J4*(J4+1)             A 306
      J1=J4                      A 307
      DO 38 I=1,N               A 308
      R=RV(I) S C=A(I) SD=DV(I) A 309
      RV(I)=R*(1.-2.*D*J2/R+C/(R*2.*J3))          A 310
      RVE=R*J2+C*J4/2.-D*J2*J2          A 311
      G(I)=G(I)+RVE            A 312
      GB(I)=G(I)                A 313
38    CONTINUE                 A 314
      GO TO 41                  A 315
C
C     DOUBLET PI ELECTRONIC STATE - ALMY AND HORSEFALL -
C
C     OH X2PI IS INVERTED F2=(-)-J=K+1/2 AND F1=(+)-J=K-1/2
C     K IS READ IN MUST CONVERT TO J INDEX FOR F2 INDEX FOR F1
C     J(PROGRAM)=K(PHYSICAL) J1(PROGRAM)=J(PHYSICAL)          A 316
                                              A 317
                                              A 318
                                              A 319
                                              A 320
                                              A 321
                                              A 322
                                              A 323
                                              A 324
                                              A 325
                                              A 326
                                              A 327
                                              A 328
                                              A 329

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29 J1=J(LJ)+(-1)**(IND-1)*.5 A 230
J2=J1+J1+J1 A 231
DO 47 I=1,N A 232
R=RV(I) A 233
D=DV(I) A 234
C=A(I) A 235
C F=ALMADA=AV/RV A 236
F=C/R A 237
C F=MU=DV/RV A 238
F=D/R A 239
R1=R+2*D+J2-.5*D A 240
RA=ALPHA**.5 A 241
R2=1+F*(4*J2+1-2*F)+F+F*(2*J2-.5)*(2*J2-.5)-F*F A 242
RA=(.25*F-F+1+(J2-.75)*R2)**.5 A 243
PARTIAL DERIVATIVE OF ALPHA = RP A 244
RP=.5/RA*(R2+(J2-.75)*(4*F+F*F*(4*J2-1)*2)) A 245
C 7=IND FOR F1 ,R=IND FOR F2 A 246
RV(I)=P1+(-1)**IND*R*RP A 247
FE=R*(J2-.75)+D*(J2*J2-.5*J2+13/16)+R*RA*(-1)**IND A 248
G(I)=G(I)+FE A 249
GR(I)=G(I) A 250
40 CONTINUE A 251
C PRINT K AND J THE ROTATIONAL QUANTUM NUMBERSS FOR THIS PROBLEM A 252
41 PRINT 71, J(LJ),J1 A 253
C A 254
C PRINT GV RV JUST CALCULATED A 255
C A 256
WRITE (6,72) CIFN(IIFN) A 257
WRITE (6,73) (G(I),I=1,N) A 258
WRITE (6,74) CIFN(IIFR) A 259
WRITE (6,75) (RV(I),I=1,N) A 260
PRINT 71, J(LJ),J1 A 261
C A 262
C FIND ZERO POINT VARIABLES A 263
C A 264
NINT=1 A 265
DO 42 I=1,6 A 266
YY(I)=I A 267
YY(I)=DV(I) A 268
YYY(I)=G(I) A 269
42 CONTINUE A 270
SIGH(1)=YY(A) A 271
NORDER=3 A 272
MPTS=6 A 273
CALL LSORTT (XY,YY,NINT,NORDER,MPTS,SIGH,ANS) A 274
RFOU1=ANS(1)+ANS(2)*(0.5)+ANS(3)*(0.25) A 275
CALL LSORTT (YY,YYY,NINT,NORDER,MPTS,SIGH,ANS) A 276
ZPTEN=ANS(1)+ANS(2)*(0.5)+ANS(3)*(0.25) A 277
RF=4.105852026/(RFOU1*ZPTEN)**.5 A 278
CALL RKF (RMIN,RMAX,VSTART,VFIN,HDED,NFIN,FV1,U,IOHK,IRHK,IPREV,IO
1PA,REGTIL,IPREG) A 279
A 280
ADDED BLOCK OF PRINT OUT A 281
REQUIRES ADDITIONAL DATA CARDS AT END OF DATA DECK A 282
DISSOCIATION ENERGY - CARDS 1 E9.2 22 A 283
DISSOCIATION PRODUCTS - CARDS 2 A10 23 A 284

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PRINT 51, (FMT(I),I=1,16) A 385
PRINT 76, (D3(I),I=1,2) A 386
D2F=D2/8066.02 A 387
PRINT 77, 7MAS1,D2,D2F A 388
PRINT 78, J(LJ),J1 A 389
PRINT 79 A 390
PRINT 80 A 391
ZE=0.0 A 392
PRINT 81, ZF,ZF,RF,ZF,BEQUIL A 393
ASTAR=1H*
PUNCH 51, (FMT(I),I=1,8)
PUNCH 82
L=0 A 394
DO 44 I=1,NFIN A 395
G2=U(I) A 396
G1=G2/8066.02 A 397
G3=G2/109737.039 A 398
RMI=RMIN(I)
RMA=RMAX(I)
RM11=RMI/.529172 A 401
RMA1=RMA/.529172 A 402
VLEV=Y1(I)
CH=VLFV-INT(VLFV) A 403
IF (CH.GT..45.AND.CH.LT..55) GO TO 43 A 404
PRINT 86, VLFV,G1,RMI,RMA,G2,ASTAR A 405
GO TO 44 A 406
43 L=L+1 A 407
LI=L-1 A 408
R1=RV(L) A 409
A1=A(L) A 410
D1=DV(L) A 411
R1I=RV1(L) A 412
G2I=G1(L) A 413
F=GR(L) A 414
E1=F/8066.02 A 415
PRINT 85, VLEV,G1,RMI,RMA,G2,R1,F,ASTAR,G2I,R1I,A1,LI A 416
PUNCH 83, LI,G2 A 417
44 CONTINUE A 418
PUNCH 84, RF,ZF A 419
DO 45 I=1,NFIN A 420
PUNCH 84, RMIN(I),U(I),RMAX(I),U(I) A 421
45 CONTINUE A 422
IF (LJ.GT.1) GO TO 46 A 423
RM=RMIN(NFIN)-.2 A 424
XMIN=AMAX1(0.,RM) A 425
XMAX=RMAX(NFIN)+1. A 426
YMAX=D2+20000. A 427
CALL MAPG (XMIN,XMAX,0.,YMAX,.1,1.,.1,1.)
CALL ABSLINE (0.,0.,0.,1.) A 428
A 429
CALL ARSVECT (1.,1.) A 430
CALL ARSVECT (1.,0.) A 431
CALL ARSVECT (0.,0.) A 432
CALL ARSVECT (0.,0.,0.05) A 433
CALL CHAROPT (0.,0.,0.,0.) A 434
CALL SYMBOL (10HRADIUS(ANGSTROMS)) A 435
A 436
A 437
A 438
A 439

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CALL ARSPFAM (.25••.02) A 440
CALL SYMBOL (2SHRKR POTENTIAL GENERATED$.) A 441
CALL ARSPFAM (.65••.02) B 442
CALL SYMBOL (FMTI) A 443
CALL ARSPFAM (.05••.4) A 444
CALL CHAROPT (0••0••1•0) A 445
CALL SYMBOL (14HENERGY(CM-1)$.) A 446
46 V(1)=GR(1) A 447
V(1001)=RF A 448
V(2001)=RF A 449
DO 47 I=1•NFIN A 450
K=I+1 A 451
V(K)=U(I)+GR(1) A 452
V(1000+K)=RMIN(I) A 453
A 454
47 V(2000+K)=RMAX(I) A 455
NPTS=NFIN+1 A 456
A 457
CALL LINES (V(1001),V(1)+NPTS) A 458
CALL LINES (V(2001),V(1)+NPTS) A 459
NL=J/LJ) A 460
A 461
CALL CHAROPT (0••0••0••0) A 462
CALL NUMBER (NL,7H2HJ=•13) A 463
48 CONTINUE A 464
CALL FRAME A 465
GO TO 1 A 466
49 CALL EXIT A 467
C A 468
50 FORMAT (I1) A 469
51 FORMAT (8A10) A 470
52 FORMAT (14.2F10.0) A 471
53 FORMAT (2I4.4X,6A10) A 472
54 FORMAT (5E10.3) A 473
55 FORMAT (E10.4•11•13•F10.4•11) A 474
56 FORMAT (RF10.0) A 475
57 FORMAT (10I3) A 476
58 FORMAT (F10.0) A 477
59 FORMAT (3F10.0) A 478
60 FORMAT (F9.2) A 479
61 FORMAT (2A17) A 480
62 FORMAT (//4H THE MASSES OF THE TWO ATOMS, BASED ON A6•6H, ARE F A 481
112•6•8H AND F10•6•6//) A 482
63 FORMAT (//4H THE REDUCED MASS OF THE TWO ATOMS, BASED ON A6•5H, A 483
1 IS F10•6•6//) A 484
64 FORMAT (6H2 THE G(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPUT A 485
1H DATA. //7H RE = F10•6•8H, WEXF =F10•4•8H, WEFY =F10•3•8H, WFZF A 486
2=F10•3•8H, WETF =F10•3) A 487
65 FORMAT (3H2 THE INPUT G VALUES, ENERGY IN A6•18H, ARE GIVEN BELOW A 488
1•//) A 489
66 FORMAT (1X10F11•3) A 490
67 FORMAT (20X,4RHVALUES OF -10, ARE TO BE FOUND BY INTERPOLATION.) A 491
68 FORMAT (6H2 THE RV(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPUT A 492
1H DATA. //7H RE = 1PF11•5•10H, ALPHAF =F11•4•10H, GAMMAF =F11•4, A 493
210H, DELTAF =F11•4•10H, EPSLNF =F11•4) A 494
69 FORMAT (3H2 THE INPUT RV VALUES, ENERGY IN A6•18H, ARE GIVEN BELOW A 495
1W•//) A 496
70 FORMAT (1X10F11•6) A 497

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71	FORMAT (4H)K= ,13.4H J= ,F4.1)	A 495
72	FORMAT (61H THE FOLLOWING NUMBERS ARE THE MODIFIED G VALUES. ENER	A 496
	1GY IN ,A6.17H ARE GIVEN BELOW.//)	A 497
73	FORMAT (1X10F11.3)	A 498
74	FORMAT (46H THE FOLLOWING ARE THE MODIFIED RV, ENERGY IN A6.//)	A 499
75	FORMAT (1X10F11.6)	A 500
76	FORMAT (1H0.6X,29HDISSOCIATION PRODUCTS ARE ,2A10)	A 501
77	FORMAT (1H0.6X,13HREDUCED MASS=,F9.5.6X,21HDISSOCIATION ENERGY =,F	A 502
	10.2.6H 1/CM=,F9.4.3H FV)	A 503
78	FORMAT (1H0.5X,17HROTATIONAL LEVEL ,4X,2HK=,15.7X,2HJ=,F5.1//)	A 504
79	FORMAT (28X,15HCALCULATED DATA,47X,17HEXPERIMENTAL DATA//)	A 505
80	FORMAT (4H V*,5X,6HGV(FV),3X,7HMIN(A),2X,7HMAX(A),3X,8HGV(1/CM)	A 506
	1.2X,8HBV(1/CM),3X,5HF(FV),3X,7HE(1/CM),4X,1H*,4X,8HGV(1/CM),3X,8HR	A 507
	2V(1/CM),3X,8HDV(1/CM),3X,8HAV(1/CM),3X,1HV//)	A 508
81	FORMAT (2X,F3.1,2X,F9.6.6X,F7.4.7X,F9.3.2X,F8.4)	A 509
82	FORMAT (11H KV,ETRIAL)	A 510
83	FORMAT (110,F10.3)	A 511
84	FORMAT (4F12.5)	A 512
85	FORMAT (1H ,F4.1.2X,F9.6.2X,F7.4.2X,F7.4.2X,F9.3.2X,F8.4.2X,F6.3.2	A 513
	1X,F7.1.4X,A1.4X,F8.2.3X,F8.4.2X,F9.3.3X,F8.2.3X,I2)	A 514
86	FORMAT (1H ,F4.1.2X,F9.6.2X,F7.4.2X,F7.4.2X,F9.3.32X,A1)	A 515
	FND	A 516-

```

SUBROUTINE RKR (RMIN,RMAX,VSTA,VFIN,HDEF,M,EV1,U,IQHK,IPHK,IPRFV,I
1
C      IOPA,REQUIL,IPREG)
2
3      RKR - FINDS TURNING POINTS FROM G(V) AND RV DATA, OR FROM CONSTANT
4      DIMENSION JV(13000), EV(13000), RV(13000), RI(13000), TEMP(13000),
5      U(13000), RMIN(13000), RMAX(13000), Y(13000), ZOC(13000), MZ(13000),
6      T(13000), IG(13000)
7
8      DIMENSION V(13000), GV(13000), RD(13000), DEV(13000), OV(13000), XG(13000),
9      YG(13000), ZG(13000), EPSH(13000), AGAUS(13000), XGAUS(13000), VSTA(13000),
10     VFIN(13000), H(13000), DEED(13000), FEND(13000), FFL(13000), ANS(13000),
11     YY(13000), XFF(13000), SIGH(13000), XY(13000), UU(13000),
12     T(13000), HT(13000), IX(13000), UX(13000)
13
14      DIMENSION DEVP(13000), OVR(13000)
15
16      COMMON Y,TEMP,JEV,EV,D,NST,NMST,D,XMIN,XMAX,INSC,NREG,NUSED,RI,NI
17      1,NS,MAXIT,FAC,ZMU,DF,WF,WFXE,WFYF,WETF,BE,ALPHAE,GAMMAE,DELT
18      2AE,VNIN,BO,NG,SREP,UUU,RV,Z,ICK,H,K,HDEF,FPSSLNF,XX,RRRRRB,ZPTEN,ML
19
20      3V,LV,PF
21
22      GFUNCF(X)=(((((WETF*X)+WFZF)*X)+WFYF)*X)-WFXE)*X)+WF)*X
23
24      PFUNCF(X)=((((((EPSLNE*X)+DELTAE)*X)+GAMMAF)*X)-ALPHAF)*X)+BF
25
26      FAC=(HPLANK*NAV/R*PI**2*C)**.5*E8/ZMU**.5
27
28      FAC=4.1257859/SORTF(ZMU)
29
30      NPROB=1
31
32      MUST=8
33
34      EV1=0.0
35
36      CALL SECOND (BEGIN)
37
38      C      TURNING POINTS FOUND FOR V = VSTA,VFIN,HDEF.
39
40      C      INTERPOLATE G(V) AND RV DATA
41
42
43      JJ=0
44
45      JK=0
46
47      IU=0
48
49      IK=0
50
51      HDEF=.01
52
53      IPREG=1
54
55      IF (IPRFV-1) 2,1,2
56
57      1   EV1=7(1)
58      WRITE (6,1) 7) MUST
59      2   DO 3 I=1,1
60      3   IF (7(1)+10.0) 2,6,6
61      4   IU=IU+1
62      TEMP(IU)=V(1)
63      5   (IU)=7(1)
64      GO TO 5
65
66      6   JJ=JJ+1
67      7   EV(JJ)=V(1)
68      8   IG(JJ)=7
69      9   IF (RV(1)+10.0) 6,7,6
70      10  IK=IK+1
71      11  RMIN(IK)=V(1)
72      12  RMAX(IK)=RV(1)
73      13  GO TO 9
74
75      JK=JK+1
76      14  EV(JK)=V(1)
77      15  IG(JK)=7
78      16  CONTINUE

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9	IF (JJ) 12,12,9	R 56
	CALL NTRPSR (TEMP,U,UEV,P1,HDFS,IJ,JJ,VNIN,VN,INSC,MREG,NUST)	R 57
	LOC=9	R 58
	IF (INSC) 97,10,97	R 59
10	DO 11 I=1,JJ	R 60
	IJ=IR(I)	R 61
	Z(IJ)=RI(I)	R 62
11	CONTINUE	R 63
12	IF (JK) 14,16,13	R 64
13	CALL NTRPSR (RMIN,RMAX,EV,P1,HDFS,IK,JK,VNIN,VN,INSC,MREG,NUST)	R 65
	LOC=9	R 66
	IF (INSC) 97,14,97	R 67
14	DO 15 I=1,JK	R 68
	IK=IR(I)	R 69
	PV(IK)=RI(I)	R 70
15	CONTINUE	R 71
16	IF (IQHK) 17,19,17	R 72
17	FV1=-GFUNCF(0.5)	R 73
	TOPFV=0	R 74
	DO 18 I=1,N	R 75
	Z(I)=GFUNCF(Y(I))+FV1	R 76
18	CONTINUE	R 77
	GO TO 22	R 78
19	INTG=INTG	R 79
	MREG=1	R 80
	N=1	R 81
	UEV(I)=0.	R 82
	HDFS=1.	R 83
	FV1=-FV1	R 84
	IF (FV1) 22,20,20	R 85
20	CALL NTRPSR (Y,Z,UEV,EV,HDFS,N,M,VNIN,VN,INSC,MREG,NUST)	R 86
	LOC=1	R 87
	IF (INSC) 97,21,97	R 88
21	FV1=FV(I)	R 89
C	FV1 NOW CONTAINS THE ZERO POINT ENERGY BY EXTRAPOLATION.	R 90
	FV1=ZPTEN	R 91
22	IF (IQHK) 22,25,22	R 92
23	FV(I)=FV	R 93
	DO 24 I=1,N	R 94
	ZV(I)=GFUNCF(Y(I))	R 95
24	CONTINUE	R 96
	GO TO 29	R 97
25	IF (TOPA) 24,27,24	R 98
26	FV(I)=BFCUL	R 99
	GO TO 29	R 100
27	CALL NTRPSR (Y,BM,UEV,EV,HDFS,N,M,VNIN,VN,INSC,MREG,NUST)	R 101
C	FV(I) NOW CONTAINS RF BY EXTRAPOLATION	R 102
	LOC=7	R 103
	IF (INSC) 97,29,97	R 104
28	V(I)=0.	R 105
	S(I)=0.	R 106
	SC(I)=FV(I)	R 107
	DO 29 I=1,N	R 108
	V(I+1)=V(I)	R 109
	S(I+1)=S(I)	R 110

```

20    RD(I+1)=PV(I)
CONTINUE
NP=N+1
1F (102EVI) 20,31,30
CONTINUE
EV1=EV1+C(2)
21  DO 22 I=2,NP
G(I)=G(I)-EV1
Y(I)=V(I)
Z(I)=G(I)
PV(I)=PV(I)
22  CONTINUE
1F (102EVI) 23,34,32
EV1=-C(2)
24  IF (NP0R=17) 37,35,27
25  M=1
EV(I)=0E
CALL NTOPSR (Z,Y,EV,DEV,H0ES,NP,M,VNIN,VM,INSC,MREG,MUST)
LOC=2
1F (1NSC) 27,36,27
NP=NP+1
Y(NP)=DEV
V(NP)=DEV
Z(NP)=0E
C(NP)=0E
PV(NP)=0E
27  M=2
Y(I)=0E
Z(I)=0E
PV(I)=PV(I)
VN=VNSTA
VN=VNIN
H0ES=H0ED
M=3
WRITE (6,102) (Y(I)+PV(I)+Z(I),I=1,NP)
WRITE (6,103) (Y(I)+PV(I)+Z(I),I=1,NP)
1F (104K) 38,42,38
M=(VN-VNSTA)/NP0+1
28  DO 29 I=1,M
DEV(I)=VNSTA+LOCATE(I-1)*NP0
DEVSP(I)=DEV(I)
PV(I)=CFLINE(DEVSP(I))
PV(I)=PV(I)
DEV(I)=DEV(I)
CONTINUE
INSC=2
29  DO 30 I=1,M
CALL NTOPSR (V,G,DEV,SV,H0ED,NP,M,VNSTA,VNIN,INSC,MREG,MUST)
LOC=2
30  WRITE (6,110) H0ES,VNIN,VM,MREG,MUST,INSC,NP,M
31  WRITE (6,111)
32  WRITE (6,112) (DEV(I)+PV(I)+Z(I),I=1,NP)
1F (104K) 37,42,37
33  DO 34 I=1,M
DEV(I)=DEV(I)

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```

43      U(1)=OV(1)          R 166
C      CONTINUE          R 167
C      INTEGRATION CONSTANTS          R 168
C
      STEP=.9          R 169
      VZ(1)=101          R 170
      VZ(2)=R          R 171
      VZ(3)=61          R 172
      IZ(1)=R          R 173
      XGAUS(1,1)=.012855071751232          R 174
      XGAUS(1,2)=.101656761293196          R 175
      XGAUS(1,3)=.237223725041896          R 176
      XGAUS(1,4)=.408282679752175          R 177
      XGAUS(1,5)=1.-XGAUS(1,4)          R 178
      XGAUS(1,6)=1.-YGAUS(1,3)          R 179
      XGAUS(1,7)=1.-YGAUS(1,2)          R 180
      YGAUS(1,8)=1.-XGAUS(1,1)          R 181
      AGAUS(1,1)=.050614269148198          R 182
      AGAUS(1,2)=.111120517226697          R 183
      AGAUS(1,3)=.156853322939044          R 184
      AGAUS(1,4)=.1812419916009181          R 185
      AGAUS(1,5)=AGAUS(1,4)          R 186
      AGAUS(1,6)=AGAUS(1,3)          R 187
      AGAUS(1,7)=AGAUS(1,2)          R 188
      AGAUS(1,P)=AGAUS(1,1)          R 189
      IZ(2)=6          R 190
      XGAUS(2,1)=.033765242999424          R 191
      XGAUS(2,2)=.160395306766868          R 192
      XGAUS(2,3)=.380690406058402          R 193
      XGAUS(2,4)=1.-XGAUS(2,3)          R 194
      XGAUS(2,5)=1.-XGAUS(2,2)          R 195
      XGAUS(2,6)=1.-XGAUS(2,1)          R 196
      AGAUS(2,1)=.085662246100598          R 197
      AGAUS(2,2)=.180380786574070          R 198
      AGAUS(2,3)=.222056057208346          R 199
      AGAUS(2,4)=AGAUS(2,3)          R 200
      AGAUS(2,5)=AGAUS(2,2)          R 201
      AGAUS(2,6)=AGAUS(2,1)          R 202
      IZ(3)=4          R 203
      XGAUS(3,1)=.060431844202974          R 204
      YGAUS(3,2)=.230009478207572          R 205
      YGAUS(3,3)=1.-YGAUS(3,2)          R 206
      YGAUS(3,4)=1.-YGAUS(3,1)          R 207
      AGAUS(3,1)=.173027422569727          R 208
      AGAUS(3,2)=.326072577431272          R 209
      AGAUS(3,3)=AGAUS(3,2)          R 210
      AGAUS(3,4)=AGAUS(3,1)          R 211
      ZG(1)=ZG(3)          R 212
      WRITE(6,113)          R 213
      DO 94 I=1,N          R 214
      TEMP1=DFV(I)          R 215
      MUS2=MUST/2          R 216
      NR=MUS2+1          R 217
      NF=N-NP+1          R 218
      113

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```

    DO 44 J=NP,NE          R 221
    IF (TEMP1-V(J)) .LT. 45,45,44          R 222
44  CONTINUE                R 223
    ISG=NE+1                      R 224
    GO TO 46                      R 225
45  ISG=J                      R 226
46  MSTA=ISG-MUS2                R 227
    VMIN=0.                         R 228
    FEG=1.                         R 229
    REG=0.                         R 230
    LT=1                           R 231
    TGD=0.                         R 232
    GDO=0.                         R 233
    FDO=0.                         R 234
    ISG=0.                         R 235
    ISB=0.                         R 236
    C
    C COMMENCE FINDING TURNING POINTS BY INTEGRATION
    C
    CALL SECOND (REGIA)           R 237
    RS=VMIN+(TEMP1-VMIN)*STEP          R 238
    IF (LT-2) 48,48,57          R 239
48  MZ=MZ(LT)                  R 240
    KM=(MZ-1)/2                  R 241
    TMIN=VMIN                  R 242
    TS=RS                  R 243
    A=(TS-TMIN)/ELDATE(MZ-1)          R 244
    MX=0.                         R 245
    IF (IOHK) 100,40,100          R 246
49  CALL NTPRSP (Y,Z,UEV,EV,A,ND,MY,TMIN,TS,INSC,MREG,MUST)
    LOC=2.                         R 247
    IF (INSC) 97,50,97          R 248
    IF (GDO) 98,51,98          R 249
50  MX=0.                         R 250
    IF (IBUK) 102,52,102          R 251
51  CALL NTPRSP (Y,Z,UEV,EV,A,ND,MY,TMIN,TS,INSC,MREG,MUST)
    LOC=4.                         R 252
    IF (INSC) 97,53,97          R 253
52  DO 55 J=1,ND          R 254
    DENO=U(J)-EV(J)          R 255
    IF (DENO) 98,99,94          R 256
53  UEV(J)=1./SQRTE(DENO)          R 257
    EV(J)=D(J)/UEV(J)          R 258
    CONTINUE                      R 259
    ESUM=UEV(1)+4.*UEV(2)+UEV(MZ)
    GSUM=EV(1)+4.*EV(2)+EV(MZ)
54  DO 56 J=2,KM          R 260
    ESUM=ESUM+4.*UEV(2+J)+2.*UEV(2+J-1)
    GSUM=GSUM+4.*EV(2+J)+2.*EV(2+J-1)
55  CONTINUE                      R 261
    EY=2.*ESUM/3.          R 262
    GEY=2.*GSUM/3.          R 263
    IF (LT-1) 96,97,98          R 264
56  TGD=(LT-1)/2          R 265
    IF (TGD-2) 99,99,99          R 266

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58      IZDO=3          R 276
59      NGAS=12(IZDO)   R 277
60      DO 60 J=1,NGAS  R 278
       XG(J)=(RS-VMIN)*YGAUS(IZDO,J)+VMIN
       UEV(J)=XG(J)
60      CONTINUE        R 281
       MST=1             R 282
       EPSH=TEMP1-XG(NGAS) R 283
       FEPS=EPSH
       IF (EPSH(1)) 93,61,62  R 284
61      IF (EPSH(2)) 93,93,62  R 285
62      IF (IQHK) 104,63,104  R 286
63      CALL NTRPSR (V,G,XG,YG,EPSP,NP,NGAS,VMIN,PS,INSC,MST,NUST)
       LOC=5             R 288
       IF (INSC) 97,64,97  R 289
64      IF (IZDO) 65,65,75  R 290
65      IF (GDO) 68,66,68  R 291
66      MST=1             R 292
       IF (IBHK) 105,67,105 R 293
67      CALL NTRPSR (Y,BV,UEV,P1,FEPS,NP,NGAS,TMIN,TS,INSC,MST,NUST)
       LOC=6             R 294
       IF (INSC) 97,68,97  R 295
68      FSUM=0.0           R 296
       GSUM=0.0           R 297
69      DO 72 J=1,NGAS    R 298
       IF (IQHK) 70,69,70  R 299
       DENO(J)=OV(J)-YG(J) R 300
70      IF (DENO(J)) 99,99,71 R 301
71      XG(J)=AGAUS(IZDO,J)/SORTE(DENO(J))
       YG(J)=P1(J)*XG(J)
       FSUM=FSUM+XG(J)
       GSUM=GSUM+YG(J)
72      CONTINUE        R 302
       IF (P1(NGAS)-P1(1)) 74,73,74  R 303
73      IZDO=1           R 304
74      RSV=RS-VMIN
       FEG2=RSV*FSUM
       GEG2=RSV*GSUM
       GO TO 78           R 305
75      FSUM=0.0           R 306
       DO 77 J=1,NGAS    R 307
       DENO=OV(J)-YG(J)
       IF (DENO) 99,99,76  R 308
76      XG(J)=AGAUS(IZDO,J)/SORTE(DENO)
       FSUM=FSUM+XG(J)
77      CONTINUE        R 309
       GSUM=P1(NGAS)*FSUM
       GO TO 74           R 310
78      IF (FEG2/FEG-1.E-6) 79,79,80  R 311
79      FDO=1.
80      IF (GEG2/GEG-1.E-6) 81,81,82  R 312
81      GDO=1.
82      IF (ABSF(FEG2/FEG1)-.9) 84,94,93  R 313
83      FDO=1.
84      IF (ABSF(GEG2/GEG1)-.9) 86,96,95  R 314
                                         R 315
                                         R 316
                                         R 317
                                         R 318
                                         R 319
                                         R 320
                                         R 321
                                         R 322
                                         R 323
                                         R 324
                                         R 325
                                         R 326
                                         R 327
                                         R 328
                                         R 329
                                         R 330

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95 GDO=1. R 231
96 LT=LT+1 R 232
97 FEG1=FEG2 R 233
98 GEG1=GEG2 R 224
99 IF (GDO) 88,87,88 R 235
100 FEG=FEG+FEG2 R 236
101 IF (GDO) 80,89,90 R 237
102 IF (GDO) 93,89,92 R 238
103 GEG=GEG+GEG2 R 239
104 VMIN=BS R 240
105 IF (IDPEG) 91,92,91 R 241
106 CALL SECOND (AFTEA) R 242
107 XTIO=(AFTEA-REGIA) R 243
108 REGIA=AFTEA R 244
109 WRITE (6,114) FEG,GEG,XTIO R 245
110 IF (LT-20) 47,47,98 R 246
111 F=FEG*FAC R 247
112 GF=GEG/FAC R 248
113 RMAX(I)=SQRTE(F*F+E*GF)+E R 249
114 RMIN(I)=RMAX(I)-2.*F R 250
115 CALL SECOND (AFTER) R 251
116 XTIO=AFTER-REGIA R 252
117 REGIA=AFTER R 253
C WRITEOUTPUTAPE6,104,TEMP1,U(I),RMIN(I),RMAX(I),XTIO,PI(NGAS) R 254
118 TEMP1I=TEMP1 R 255
119 WRITE (6,115) TEMP1I,U(I),RMIN(I),RMAX(I),XTIO,PI(NGAS),F,GF R 256
120 CONTINUE R 257
121 DO 95 I=1,N R 258
122 Z(I)=Z(I+1) R 259
123 Y(I)=Y(I+1) R 260
124 RV(I)=RV(I+1) R 261
125 CONTINUE R 262
126 WRITE (6,113) R 263
127 RETURN R 264
128 ZOC(1)=6H FV1 R 265
129 ZOC(2)=6HG(LFV) R 266
130 ZOC(3)=6HS,P,FV R 267
131 ZOC(4)=6HC,P,FM R 268
132 ZOC(5)=6HD,P,FM R 269
133 ZOC(6)=6HN,P,FM R 270
134 ZOC(7)=6H RV1 R 271
135 ZOC(8)=6H2 FILL R 272
136 ZOC(9)=6H2RV2FILL R 273
137 WRITE (6,116) ZOC(LOC),U(I) R 274
138 INTG=1 R 275
139 GO TO 94 R 276
140 WRITE (6,117) R 277
141 INTG=1 R 278
142 GO TO 96 R 279
143 INTG=1 R 280
144 WRITE (6,119) R 281
145 GO TO 96 R 282
146 MX=0 R 283
147 DO 101 J=1,MQ R 284
148 UEV(J)=TMIN+ELCATH(J-1)*A R 285

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101   UV(J)=GFUNCF(UFV(J))          R 386
      CONTINUEF
      GO TO 50
102   MX=MQ
      DO 103 J=1,MQ
      UFV(J)=TMIN+FLOATF(J-1)*A
      RI(J)=RFUNCF(UFV(J))
103   CONTINUEF
      GO TO 53
104   CALL DGUNC (XG,PENO,NCAS,TEMP1)
      GO TO 64
105   DO 106 J=1,NCAS
      RI(J)=RFUNCF(UFV(J))
106   CONTINUEF
      GO TO 68
C
107   FORMAT (20H0 NUSED IN PFSRKR = I2,I4)
108   FORMAT (32H0 THE G(V) VALUES USED BELOW ARE//,6X,6(2X,1HV7X,1HG10Y
109   1),/,6(F10.1,F11.4)))
110   FORMAT (33H0 THE RV(V) VALUES USED BELOW ARE//,6X,6(2X,1HV6X,2HRV1
111   1PX),/,6(F10.1,F11.7)))
112   FORMAT (16H0HDFS=1PF15.7,7H, VMIN=E15.7,5H, VN=E15.7,7H, VRG=I5/9X
113   1,7H, NUST=I5,7H, INSC=I5,4H, N=I5,4H, M=I5)
114   FORMAT (54H0 OUTPUT V,G--LEVELS AT WHICH TURNING POINTS ARE FOUND/
115   1/,6X,6(2X,1HV7X,1HG10Y)/)
116   FORMAT (6(F10.1,F11.4))
117   FORMAT (1H1)
118   FORMAT (6X,6HFFG = 1PF15.7,8H, GEG = E15.7,10X,SHREQUIRED OFP8.3,9
1H SECONDS.)
119   FORMAT (10H0 FOR V = F5.1,3X,6H G = F10.2,14H 1/CM, RMIN = F10.7,
120   112H AND RMAX = F10.7,27H ANGSTROMS. THIS REQUIRED FB.2,9H SECONDS
121   2,20X,12H ALSO, BV = F12.7/20X,49H THE KLEIN ACTION INTEGRALS F AND
122   G ARE EQUAL TO 2E15.0///)
123   FORMAT (26H0 NTRPDP UNSUCCESSFUL FOR A6+11H, WHEN U = E16.8)
124   FORMAT (21H0 TFG REACHED MAXIT )
125   FORMAT (22H0 PENO IS NOT POSITIVE)
      END

```

```

C SUBROUTINE NTRPSR (XJ,YJ,YO,YO,XN,N,K,XMIN,XMAX,INSC,MREG,NUSED)
C NTRPSR - INTERPOLATION PROGRAM (BY SUCCESSIVE RANGES) SINGLE PREC.
C
C THE METHOD OF LAGRANGE IS USED. THE INPUT POINTS NEED NOT BE
C EQUALLY SPACED. THERE ARE TWO MODES OF INPUT AVAILABLE. THE
C FIRST OCCURS WHEN M = 0. THE ABSCISSAE ARE THEN GENERATED FROM
C XMIN-XMAX, AND XH. AT EXIT M = NO. OF POINTS FOUND, AND XO
C CONTAINS THE ABSCISSAE. M WILL BE CHECKED TO INSURE THAT THE
C DIMENSION IS NOT EXCEEDED. MDIMM = THE DIMENSION OF THE XO, YO
C ARRAYS. THE SECOND MODE OCCURS WHEN M IS POSITIVE. THE M
C ABSCISSAE ARE THEN ASSUMED TO HAVE BEEN GENERATED PRIOR TO
C ENTRY. THE STARTING INDEX FOR THE OUTPUT ARRAY MUST BE
C SPECIFIED. THE FIRST POINT FOUND WILL BE AT XO(MREG). XH MUST
C BE GIVEN SINCE THE ORDINATE FOR ANY POINT CLOSER THAN .01*XH TO
C AN INPUT POINT IS TAKEN AS THAT FOR THE INPUT POINT. -NUSED- IS
C THE NUMBER OF POINTS USED FOR EACH INTERPOLATED POINT. *NUSED*
C MUST BE EVEN AND LESS THAN OR EQUAL TO -N-. NUSED = 8 IS
C SUGGESTED. ANY POINT FARTHER THAN NUSED/2 POINTS FROM EITHER END
C IS FOUND FROM THE NUSED/2 ON EACH SIDE. NTRPSR WILL SCALE AND
C RESCALE IN ORDER TO AVOID OVERFLOW. IF THE FIRST SCALING DOES
C NOT SUCCEED, NTRPSR WILL TRY UP TO 7 TIMES MORE BEFORE RETURNING
C IN THE ERROR MODE. (INSC = 1)
C INPUT IS X1,Y1,(XO),YH,N,M,(XMIN),(XMAX),MREG,NUSED.
C OUTPUT IS (XO),YO,INSC.
C INSC = 0 IF PROGRAM WAS SUCCESSFUL. IF NOT, INSC = 1.
C
C DIMENSION XI(200), YI(200), XO(3000), YO(3000), XJ(200), YJ(200),
C INUMB(200)
C MDIMM=3000
C XMAX=XMAX
C XMIN=XMIN
C XH=ABSE(XH)
C M=K
C IRFV=0
C IRFX=0
C M IS ZERO, IF XH, XMIN, XMAX ARE TO BE USED. IF M IS NOT = TO
C ZERO, THEN XO(I), I = 1,M WILL BE USED AS ABSCISSA.
C IF (M) 32,1,6
C M=XINTE(ABSE((XMAX-XMIN)/XH))+1
C IF M IS MORE THAN DIMENSION OF XO, RETURN IN ERROR MODE.
C IF (M+MREG-MDIMM-2) 2,13,33
C ME=MREG+M-1
C IF (XMAX-XMIN) 3,4,4
C XMIN=XMAX
C XMAX=XMIN
C IRFV=1
C DO 5 I=MREG,ME
C YO(I)=FLOATE(I-MREG)*XH+XMIN
C CONTINUE
C DO 7 I=1,M
C XI(I)=XJ(I)
C CONTINUE
C ME=MREG+M-1
C MSTA=MREG
C MIST=MUSED/2

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NS=NUST+1          C 56
NF=N-NS+1          C 57
NFP=NF+1          C 58
DO 9 I=NS,NFP    C 59
NUMR(I)=0          C 60
CONTINUE
IF (XO(MF)-XO(MREG)) 0,11,11   C 61
9  M2=M/2          C 62
M2F=MREG+M2-1      C 63
DO 10 I=MREG,M2F   C 64
K=MF+MREG-1        C 65
TEMP=XO(I)
XO(I)=XO(K)
XO(K)=TEMP
10 CONTINUE
IREV'-1           C 70
11 IF (XI(N)-XI(1)) 12,14,14   C 71
12 N2=N/2          C 72
DO 13 I=1,N2      C 73
K=N+1-I          C 74
TEMP=XJ(I)
TEMS=YJ(I)
XJ(I)=XJ(K)
YJ(I)=YJ(K)
XJ(K)=TEMP
YJ(K)=TEMS
13 CONTINUE
IREX=1            C 82
14 IF (NF-NS) 10,15,15       C 83
15 DO 16 J=MREG,MF         C 84
DO 17 I=NS,NF           C 85
IF (XO(J)-XI(I)) 16,16,17   C 86
16 NUMR(I)=NUMR(I)+1     C 87
GO TO 18
17 CONTINUE
NUMR(NFP)=NUMR(NFP)+1     C 88
18 CONTINUE
GO TO 20
19 NUMR(NFP)=''          C 89
20 M=C
DO 24 L=NS,NFP         C 90
IF (NUMR(L)) 24,24,21     C 91
21 M=NUMR(L)
NSTA=L-NUST
GO TO 35
22 IF (INSC) 24,22,24     C 92
23 NSTA=MSTA+M          C 93
CONTINUE
24 K=MSTA-MBEG
IF (IREV) 28,22,26     C 94
25 M2F=K/2+MREG-1       C 95
DO 27 I=MREG,M2F       C 96
J=MF+MREG-1
TEMP=XO(I)
TEMS=YO(I)

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XO(I)=YO(J) C 111
YO(I)=YO(J) C 112
YO(J)=TEM'D C 113
YO(J)=TEM'S C 114
27 CONTINUE C 115
28 IF (IREXY) 21,21,29 C 116
29 DO 30 I=1,12 C 117
J=N-1-2 C 118
J=N+1-I C 119
TEM'D=XJ(I) C 120
TEM'S=YJ(I) C 121
YJ(I)=XJ(J) C 122
YJ(I)=YJ(J) C 123
YJ(J)=TEM'D C 124
YJ(J)=TEM'S C 125
30 CONTINUE C 126
31 RETURN C 127
32 WRITE (6,51) C 128
INSC=1 C 129
GO TO 25 C 130
33 H=(XMAX-XMIN)/FLOAT(MONMM-MREG) C 131
WRITE (6,52) H C 132
INSC=1 C 133
GO TO 25 C 134
34 WRITE (6,52) L C 135
GO TO 25 C 136
35 NCON=1 C 137
RFIA=1.414214 C 138
NFIN=MSTA+NUSED-1 C 139
DO 36 I=MSTA,NFIN C 140
XI(I)=XJ(I) C 141
YI(I)=YJ(I) C 142
CONTINUE C 143
MSTA1=MSTA+1 C 144
YSCALE=(YI(NFIN)-YI(MSTA))/10. C 145
YMAX=YI(MSTA) C 146
YMIN=YI(MSTA) C 147
DO 37 I=MSTA1,NFIN C 148
YMAX=YMAX/YI(I) C 149
YMIN=YMIN/YI(I) C 150
CONTINUE C 151
YSCALE=YMAX-YMIN C 152
DO 38 I=MSTA,NFIN C 153
XI(I)=XI(I)/YSCALE C 154
YI(I)=(YI(I)-YMIN)/YSCALE+.5 C 155
CONTINUE C 156
XH=ADSF(XH)/YSCALE C 157
NFIN=MSTA+NUSED-1 C 158
MTA=MSTA C 159
39 EPSIL=.5*YH C 160
DO 40 IT=MSTA,NFIN C 161
XO(IT)=YO(IT)/YSCALE C 162
YO(IT)=2.0 C 163
DO 41 IT=MSTA,NFIN C 164

```

```

C FIND X0(I1)-XI(I1) FOR NUMERATOR AND CHECK FOR NEARNESS. C 165
YNUM=X0(I1)-XI(I1)
IF (ABS(XNUM))=EPSILY 40+42+41 C 166
C 167
40 YO(I1)=YI(I1) C 168
GO TO 45 C 169
C 170
C PNUM = PRODUCT OF ALL YNUM C 171
41 PNUM=PNUM*YNUM C 172
C 173
C CONSTRUCT DENOMINATOR AND SUM C 174
42 PDEN=1.0 C 175
DO 43 J=NSTA,NFIN C 176
IF (I-J) 42+42+42 C 177
42 PDEN=(XI(I1)-XI(J1))*PDEN C 178
IF QUOTIENT OVERFLOW 47+43 C 179
43 CONTINUE C 180
DEN=PDEN*YNUM C 181
YO(I1)=YI(I1)/DEN+YO(I1) C 182
IF ACCUMULATOR OVERFLOW 50+44 C 183
44 CONTINUE C 184
YO(I1)=YO(I1)*PNUM C 185
45 YO(I1)=(YO(I1)-.5)*YSCALE+YMIN C 186
XO(I1)=YO(I1)*XSCALE C 187
46 CONTINUE C 188
INSC=0 C 189
GO TO 22 C 190
47 WRITE (6,54) NCON,XSCALE C 191
WRITE (6,55) II,I,J C 192
NCON=NCON+1 C 193
DO 48 I=NSTA,NFIN C 194
XI(I)=XI(I)/REFA C 195
48 CONTINUE C 196
XO(I1)=XO(I1)*XSCALE C 197
MTA=II C 198
XH=XH/REFA C 199
XSCALE=XSCALE*REFA C 200
IF (NCON-B) 39+39+40 C 201
49 INSC=1 C 202
GO TO 22 C 203
50 WRITE (6,56) C 204
INSC=1 C 205
GO TO 22 C 206
C 207
51 FORMAT (44HC ERROR IN INPUT TO NTRPSR. N IS NEGATIVE. ) C 208
52 FORMAT (58HC ERROR IN INPUT TO NTRPSR. MINIMUM ALLOWABLE TRACING C 209
11S 1PE12.3) C 210
53 FORMAT (43H0 INTPL WAS UNABLE TO INTERPOLATE IN RANGE I2) C 211
54 FORMAT (8H NCON =I2,11H, XSCALE = F10.7) C 212
55 FORMAT (26H OVERFLOW OCCURRED AT II=I4,4H I=I2,4H J=I2) C 213
56 FORMAT (48HC ACCUMULATOR OVERFLOW. DEN MUST BE TOO SMALL. ) C 214
END C 215-

```

```

SUBROUTINE DGUNC (XG,DENO,NGAS,TEMP1)          D   1
C      FINDS G(V) - G(V-X)                         D   2
      DIMENSION XG(20), DENO(20)                   D   3
      DIMENSION UEV(2000), EV(3000), BV(200), RI(3000), TEMP(200), U(200
100, V(200), Z(200)
      COMMON Y,TEMP,UEV,EV,Q,NST,N,M,XMIN,XMAX,INSC,MBEG,NUST,RINT,
1NS,MAXIT,FACM,ZNU,DF,WEXF,WFYF,WZEF,WETE,BF,ALPHAF,GAMMAF,DELTA
2E,VNIN,BQ,NO,SDEP,U,PV,Z,ICK,H,K,HDFS,EPSSLNE
      V=TEMP1
      VA=V*V
      VR=VA*V
      VC=VR*V
      DO 1 I=1,NGAS
      Y=TEMP1-XG(I)
      X=Y
      XA=X*X
      XB=XA*X
      XC=XB*X
      DENO(I)=WE*X+(XA-2.*V*X)*WEXF+((VA*X-V*XA)*3.+XB)*WFYE+((VB*X+V*XR
1)*4.-6.*VA*XA-XC)*WEZE+((VC*X-V*XC)*5.+((VA*XB-VB*XA)*10.)*WETE
1
      CONTINUE
      RETURN
      END

```

APPENDIX II
COMPUTER PROGRAM FRANKON

The program FRANKON was used at AFWL to calculate Franck-Condon factors, r centroids, r^2 centroids. A listing of this program is included in this appendix along with an explanation of the input data and a sample data deck.

1. INPUT DATA

The reduced mass of the molecule or the mass of each atom is needed. These can be based on either C_{12} or O_{16} . A good source for reduced masses based on O_{16} is Herzberg (Ref. 31). The vibrational potential of the lower electronic state and the vibrational potential of the upper electronic state is read into the program. The value of the internuclear separation r and the potential $v(r)$ may be read in any one of several different units. The potential to be read in can be obtained from the output of program TURNGPT or it can be taken from potentials which have been published. There is also the option of generating an analytic potential by programming the desired expressions and putting these in subroutine POTGEN.

Also needed are the dissociation energies of the upper and lower electronic states and the energies of the various vibrational levels for which one wishes to calculate Franck-Condon factors. The Franck-Condon factors can be calculated for any desired rotational level by specifying appropriate values for JRRTL, JRROTU. The energies of the rotationless vibrational levels are then adjusted by adding the appropriate rotational energy given by

$$E_R = \left\{ Be + \alpha_e(v+\frac{1}{2}) + \gamma_e(v+\frac{1}{2})^2 \right\} \frac{\frac{J(J+1)}{h N_o \mu}}{\left(\frac{8\pi^2 c a_o^2}{\mu} \right)}$$

where the constants Be , α_e , γ_e are read in for the lower and upper states. The separation of the minimums of the two states, T_e , is also read in.

2. DATA DECK

As in the case of program TURNGPT, Zare has made extensive use of comment cards in program FRANKON and little or no explanation is needed to explain how to set up the data deck.

Card Number

1	ITEST I1	1 in column one if problem is to follow
2	Title 72H1	carriage control in column 1, name of problem in columns 1-72
3	IIMS, ZMAS1, ZMAS2, I4, 2F10.0	IIMS = 1 mass based on C = 12 IIMS = 2 mass based on O = 16 ZMAS1 mass of first atom (reduced mass of molecule) ZMAS2 mass of second atom (or zero when using reduced mass)
(for lower state)		
4	IIRA, IIEN, N(IKON)	IIRA = units used for internuclear separation
	3I4	IIRA = 1 atomic units (a_0) IIRA = 2 Angstrom units (\AA)
		IIEN = units used for energy
		IIEN = 1 atomic units (hartree)
		IIEN = 2 1/cm (kayser)
		IIEN = 3 electron volt
		N(IKON) = number of data points for potential to be read in
5 through 5+N(1)	XI, YI Format in columns 13-72 of Card 4	XI - internuclear separation in units at IIRA YI - energy of corresponding point of potential in units of IIEN

Card Number

6+N(1)	NDE, DE(IKON) I4, F10.0	NDE = 0 if zero point of the potential is at R = ∞ NDE = 1 if zero point of the potential is at R = R_e
7+N(1)	XMIN, XMAX, XH, IIRA 3F100, I4	XMIN, XMAX the minimum and maximum value of internuclear separation at which the wave functions were calculated, with mesh spacing of XH all in units of IIRA
8+N(1)	NL, IIEN, NET 3I4 Formats for next card	NL - number of expected energy levels with units of IIEN NET = 0 zero of potential at R = ∞ NET = 1 zero of potential at R = R_e
9+N(1)	KV(I,IKON), ETRIAL (I,IKON)	KV - the vibrational level ETRIAL - energy of the vibrational level KV(IKON) in number
(for upper state)		
10+N(1)	IIRA, IIEN, N(IKON) same	Same as for lower state
11+N(1)	XI, YI	Potential for upper state; same description as lower state N(2) in number
11+N(1)+N(2)	through	
12+N(1) +N(2)	NDE, DE(IKON) Same	Same as for lower state
13+N(1) +N(2)	XMIN, XMAX, XH, IIRAI	Same as for lower state
14+N(1) +N(2)	NL (IKON) IIEN1, NET	Same as for lower state
15+N(1) +N(2)	KV (I, IKON) ETRIAL (I, IKON)	Same as for lower state
16+N(1) +N(2)	NI, NS, IPSIQ, MAXIT, EPS 4I4, E10.0	NI - 1 prints iterations, otherwise not

Card Number

Card 16 (cont'd)

17+N(1)
+N(2)JROTL, JROTU
2I3NS = 1 prints wavefunctions every
IPSIQ points18+N(1)
+N(2)BE1, AE1, GE1,
BE2, AE2, GE2
6E10.3NS = 33 prints eigenvalues and
node count19+N(1)
+N(2)TE
E10.3MAXIT - maximum number of times
SCHR will try and satisfy
convergence criterion

EPS - convergence criterion

lower and upper rotational levels
respectivelyrotational constants for lower
and upper states20+N(1)
+N(2)NPOT
I3TE - relative difference in
energy (units of 1/cm) of
the lower and upper statespotential printed every NPOT
points21+N(1)
+N(2)

Blank

NOT REPRODUCIBLE

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C UNITS FOR THE MIN AND MAX DISTANCES AND THE SPACING XH.          A 56
C READ 80, XMINTM,XMAXTM,XHTEM,IIRAI      A 57
C NEXT TWO CARDS ARE THE VALUES OF J FOR THE LOWER AND UPPER STATE   A 58
C READ 81, IJL01,IJU01      A 59
C
C NEXT CARD IN DATA HAS IIRAI, IJEN, AND THE NUMBER OF POINTS, EACH     A 60
C IN 14 FORMAT, AS WELL AS THE FORMAT STATEMENT WHICH CONTROLS THE    A 61
C READING OF THE POINTS (IN COLUMNS 19-72)--FOR EXAMPLE--(4E16.8).    A 62
C IJEN = 1, ENERGY IS IN ATOMIC UNITS. (1 A.U. = 27.1961 F.V.)      A 63
C IJEN = 2, ENERGY IS IN 1/CM.           A 64
C IJEN = 3, ENERGY IS IN ELECTRON VOLTS. (1 F.V. = 9065.62 1/CM)    A 65
C IIRAI = 1, DISTANCE IS IN ATOMIC UNITS. (1 A.U. = .529166 ANG.)   A 66
C IIRAI = 2, DISTANCE IS IN ANGSTROM'S.        A 67
C FOLLOWING CARDS CONTAIN THE INPUT POTENTIAL POINTS.                 A 68
C IF IT IS DESIRED TO USE A FUNCTION TO GENERATE THE WHOLE            A 69
C POTENTIAL CURVE, THE FIRST 12 COLUMNS OF THE IIRAI, ETC., CARD       A 70
C MUST BE BLANK. A HOLLERITH TEXT MUST BE PUNCHED IN 19-72, AS        A 71
C IT WILL BE PRINTED. THE NEXT CARD IN SUCH A CASE CONTAINS          A 72
C XMINTM,XMAX,ETC.          A 73
C
C UPPER STATE IS READ IN FIRST, LOWER STATE LAST.                   A 74
C THE SAME VALUE OF IJEN,IIRAI,NDF,XH,XMIN,XMAX,IIRAI,NET             A 75
C +IJEN1 MUST BE USED FOR BOTH THE GROUND AND UPPER STATE          A 76
C IJKON=2          A 77
3 READ 82, IIRAI,IJEN,NIKON,(ITERMT(1),I=1,10)                  A 78
XMINTM,XMINTEM          A 79
XMAX=XMAXTEM          A 80
XH=XHTEM          A 81
NIKON=(NIKON)          A 82
READ ITERMT,(X1(I),X2(I),I=1,NIKON)          A 83
NODEN=(NIKON)/2          A 84
N2DEN=D2I          A 85
READ ITERMT, X1(N2D),X2(N2D),DD0,DD01          A 86
I1=1,MEN2D          A 87
DD = 1,I=1,DD0          A 88
I1=1,I1=1          A 89
I2=I1+1          A 90
READ ITERMT, X1(I1),X2(I1),X3(I1),X4(I1)          A 91
M1(I1)=M1(I1)          A 92
CONTINUE          A 93
C
C NEXT CARD CONTAINS NDF AND THE DISSOCIATION ENERGY WHERE NDF IS      A 94
C ZERO IF ZERO PT OF POTENTIAL CURVE IS AT INFINITY, OR ONE IF AT     A 95
C INFINITE POTENTIAL. DISSOCIATION ENERGY HAS SAME UNITS AS POTENTIAL. A 96
C
C READ 83, NDF,DE(IKON)          A 97
C
C NEXT CARD HAS NO. AND IEN OF EXPECTED ENERGY LEVELS, AND NET          A 98
C WHICH HAS THE SAME INTERPRETATION FOR ETrial(I) AS NDF DOES FOR     A 99
C THE POTENTIAL CURVE ABOVE.          A 100
C IT ALSO CONTAINS THE VARIABLE FORMAT FOR READING ENERGY LEVELS     A 101

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C READ RA, NLTKON,ITEM1,NET,(DIENT(I),I=1,10) A 111
C NLTKONEN,I,TKON) A 112
C READ IN ENERGY LEVELS A 113
C READ DIENT, (KV(I),ETRIAL(I),I=1,NLTKON) A 114
C READ IN THE EXPERIMENTAL RV + CALLED RVE A 115
C READ RA, (RVE(I),I=1,NLTKON) A 116
C DOING FIRST FOR THE UPPER STATE AND THEN THE LOWER STATE, SCHRÖDINGER A 117
C EQUATION USING THE FOLLOWING METHOD A 118
C D2 M1 SCHR MODIFIED FOR THE 709/7090/7094 IS DESCRIBED IN A 119
C D. N. ZARE AND J. K. CASHION, NCRL-10881, 1962 A 120
C FOR THIS PROGRAM THE CONSTANTS ARE USED AS FOLLOWS A 121
C IF NI = 16 PRINTS ITERATIONS, OTHERWISE NOT A 122
C IF NC = 16 PRINTS WAVEFUNCTION EVERY 1000 POINTS, OTHERWISE NOT A 123
C IF NS = 32 PRINTS EIGENVALUES AND NODE COUNT A 124
C EPS IS THE CONVERGENCE CRITERION A 125
C EPS IS IN THE SAME UNITS AS THE POTENTIAL CURVE A 126
C MAXIT IS THE MAXIMUM NUMBER OF TIMES SCHR WILL TRY TO SATISFY THE A 127
C CONVERGENCE CRITERION A 128
C
C LLIM=100 A 129
C KLIM=2 A 130
C READ RA, NI,NC,IPSIO,MAXIT,EPS A 131
C
C NEXT CARD CONTAINS NROT. A 132
C THE POTENTIAL IS PRINTED AT EVERY NROT POINT. A 133
C NROT = 50 IS SUGGESTED TO THE USER. A 134
C
C READ RI, NROT A 135
C
C THIS TERMINATES COMMENT CARDS ON THE PREPARATION OF DATA. A 136
C IF NO FURTHER PROBLEMS FOLLOW, REMEMBER TO ADD A BLANK CARD TO THE A 137
C DATA DECK A 138
C
C
C OIPAI(1)=6HA011, A 139
C OIPAI(2)=6HAC007, A 140
C OIFN(1)=6HA011, A 141
C OIFN(2)=6H11/CM A 142
C OIFN(3)=6HF0V, A 143
C OIMI(1)=6HC12=12 A 144
C OIMI(2)=6H016=16 A 145
C
C OUTPUT IS IN WAVE NUMBERS AND ANGSTROEM. A 146
C PRINT HEADING A 147
C
C PRINT 79, TITLE A 148
C
C PRINT RI, NROT, OPOTH A 149
C PRINT THE MASSES AND THEIR UNITS. A 150
C
C IF (ZMAC2) .NE. 0 A 151

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5 PRINT 87, QINS(1IMS),ZMAS1,ZMAS2 A 166
6 GO TO 7 A 167
6 PRINT 88, QINS(1IMS),ZMAS1 A 168
7 CONTINUE A 169
C
C PRINT THE INPUT POTENTIAL, THE DISSOCIATION ENERGY, AND UNITS. A 170
C IF READ IN. A 171
C
C PRINT 90, QIPAI(1TRA),QIFEN(1EN) A 172
C NIKON=N(1KON) A 173
C PRINT 90, (X1(I),Y1(I),I=1,NIKON) A 174
C PRINT 91, DF(1KON) A 175
C PRINT 92, XMIN,XMAX,XH,QIPAI(1TRA) A 176
C
C PRINT THE TRIAL ENERGY LEVELS AND THEIR UNITS. A 177
C
C PRINT 93, QIFEN(1EN), (KV(I),FTRIAL(I),I=1,NL1KON) A 178
C
C PRINT THE CONVERGENCE CRITERION. A 179
C
C PRINT 94, EPS,QIFEN(1EN) A 180
C
C PRINT HEADING A 181
C PRINT 78, TITLE A 182
C PLOTTING GENERATED POTENTIALS... A 183
C
C IF (ZMAS2) 8,8,0 A 184
8 ZMU=ZMAS1 A 185
GO TO 10 A 186
9 ZMU=ZMAS1+ZMAS2/(ZMAS1+ZMAS2) A 187
10 ZIMS(1)=1.0 A 188
ZIMS(2)=.0006784 A 189
ZIRAI(1)=1.0 A 190
ZIRAI(2)=1.000746 A 191
ZM1=ZMU*ZIMS(1)MS1 A 192
ZIFEN(1)=ZM1*3.643668E3 A 193
ZIFEN(2)=ZM1*1.6610826E-2 A 194
ZIFEN(3)=ZM1*1.330776E2 A 195
FACTM=60.201702/ZMU A 196
N2=EN(2) A 197
NL2=NL(2) A 198
IND=N(1KON) A 199
DO 11 I=1,IND A 200
Y1(I)=Y1(I)*ZIFEN(1EN) A 201
Y1(I)=Y1(I)*ZIPAI(1TRA) A 202
CONTINUE A 203
11 DF=DF+ZIFEN(1EN) A 204
DF(2)=DF(2)+ZIFEN(1EN) A 205
YMIN=XMIN*ZIPAI(1TRA) A 206
YMAX=YMAX*ZIPAI(1TRA) A 207
YH=XH*ZIPAI(1TRA) A 208
EPS=EPS+ZIFEN(1EN) A 209
INDL=NL(1KON) A 210
DO 12 I=1,INDL A 211
FTRIAL(I)=FTRIAL(I)+ZIFEN(1EN)

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12  CONTINUE          A 221
CALL POTEST          A 222
C   CHECK FOR RESCALING OF POTENTIAL TO ZERO AT R=INFINITY A 223
IF (NDF) 74,15,13    A 224
13  DO 14 I=1,M      A 225
V(I)=V(I)-DF(IKON)  A 226
14  CONTINUE          A 227
15  IF (NFT) 71,18,16 A 228
16  DO 17 I=1,INDL   A 229
FTRIAL(I)=FTRIAL(I)-DE(IKON) A 230
17  CONTINUE          A 231
18  DO 19 I=1,INDL   A 232
FCALC(I)=FTRIAL(I)  A 233
19  CONTINUE          A 234
C
C   PRINT THE POTENTIAL CURVE GENERATED (ANGSTROMS AND 1/CM) A 235
C 222 WRITE(11,ISTATF,IKON,M)          A 236
C  BUFFER OUT(1:1)(XO(1),XO(M))        A 237
C 135 CONTINUE          A 238
C  IF(UNIT,1)135,240,240          A 239
C 240 BUFFER OUT(1:1)(V(1),V(M))        A 240
PRINT 95
NPOT4=NPOT#4          A 241
NPOT5=NPOT#5          A 242
DO 26 I=1,M,NPOTS    A 243
IF (I4-I-NPOT4) 20,21,21          A 244
20  JFIN=(I4-I)/NPOT          A 245
IF (JFIN) 27,27,22          A 246
21  JFIN=5          A 247
22  DO 23 J=1,JFIN          A 248
IPRN=I+NPOT*(J-1)          A 249
XPRN(J)=XO(IPRN)*.529146  A 250
VPRN(J)=(V(IPRN)+DF(IKON))*FACTM A 251
23  CONTINUE          A 252
IF (VPRN(1)-1,F6) 25,24,24          A 253
24  PRINT 96, (XPRN(J),VPRN(J),J=1,JFIN),IPRN          A 254
GO TO 26          A 255
25  PRINT 97, (XPRN(J),VPRN(J),J=1,JFIN),IPRN          A 256
26  CONTINUE          A 257
27  MTEMO=M          A 258
LLK=0          A 259
LK=0          A 260
C   FIND THE ENERGY LEVELS THROUGH USE OF SCHR.          A 261
DO 40 I=1,M!IKON          A 262
CALL SCHRO (KV(I),FCALC(I))          A 263
IF (ISCHR-1,1) 29,28,71          A 264
28  LLK=LLK+1          A 265
IF (LLK=L,LIM) 29,20,72          A 266
29  M=MTEMO          A 267
DO 30 J=1,M          A 268
XO(J)=(J-1)*XH+XMIN          A 269
RVSUM=S(1)**2/XO(1)**2+4.*S(2)**2/XO(2)**2+S(M1)**2/XO(M)**2          A 270
KSIMD=M-1          A 271
DO 31 J=2,KSIMD,2          A 272
RVSUM=2.*S(J)**2/XO(J)**2+4.*S(J+1)**2/XO(J+1)**2+RVSUM          A 273
          A 274
          A 275

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31 CONTINUE A 276
C ALSO WRITE WAVEFUNCTION ONTO TAPE A 277
C WRITE(I)IKON,NLIKON,I,M A 278
C IKON-POTENTIAL,NLIKON-NUMBER OF VIBRATIONAL LEVELS FOR A 279
C POTENTIAL IKON,I-NUMBER OF THE LEVEL,M-NUMBER OF POINTS AT WHICH A 280
C WAVEFUNCTION IS TABULATED A 281
C BUFFER OUT (I,1)(S(1),S(M)) A 282
C GO TO (33,32), IKON A 283
C PUT WAVEFUNCTION INTO EXTENDED CORE FOR LATER USE A 284
32 INFC=1+(I-1)*M A 285
CALL WRITEC (S(1),INFC,M) A 286
GO TO 30 A 287
33 DO 38 IK=1,NL2 A 288
INFC=1+M*(IK-1) A 289
CALL READFC (SU(1),INFC,M) A 290
DO 34 J=1,M A 291
XO(J)=(FLOAT(J-1)*XH+XMIN)*SU(J) A 292
CONTINUE A 293
CALL SIMP (S,SU,M,XH,RESULT(I,IK)) A 294
CALL SIMP (S,XO,M,XH,PCNTPD(I,IK)) A 295
A=XMIN A 296
DO 35 J=1,M A 297
XO(J)=A*XO(J) A 298
A=A+XH A 299
35 CONTINUE A 300
CALL SIMP (S,XO,M,XH,PPCN(I,IK)) A 301
A=XMIN A 302
DO 36 J=1,M A 303
XO(J)=A*XO(J) A 304
A=A+XH A 305
36 CONTINUE A 306
CALL SIMP (S,XO,M,XH,PRRCN(I,IK)) A 307
A=XMIN A 308
DO 37 J=1,M A 309
XO(J)=A*XO(J) A 310
A=A+XH A 311
37 CONTINUE A 312
CALL SIMP (S,XO,M,YH,PRPRM(I,IK)) A 313
38 CONTINUE A 314
39 RVF(I)=FACM*RSIM*XH/3. A 315
FCALC(I)=DF(IKON)*FACM+FCALC(I) A 316
PRINT 99, FCALC(I),RVF(I) A 317
40 CONTINUE A 318
PRINT 78, TITLE A 319
PRINT 99, LLK A 320
PRINT 100, XSTATE(IKON) A 321
PRINT 101 A 322
DO 42 I=1,NLIKON A 323
ETRIAL(I)=(ETRIAL(I)+DF(IKON))*FACM A 324
DIFE=FCALC(I)-ETRIAL(I) A 325
IF (I-1) 42,42,41 A 326
42 DGT=ETRIAL(I)-ETRIAL(I-1) A 327
DGC=FCALC(I)-FCALC(I-1) A 328
DIFDE=DGC-DGT A 329
PRINT 102, DGT,DGC,DIFDE A 330

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42 PRINT 103, KV(I), FTRIAL(I), FCALC(I), DIFF      A 221
43 CONTINUE
44 PRINT 104, XSTATE(1KON)
45 PRINT 105
46 DO 44 I=1,NL1KON
47 PRINT 106, KV(I), PVE(I), PVE(I)
48 CONTINUE
49 GO TO 146,48, 1KON
50 1KON=1
51 GO TO 3
52 CONTINUE
53 DO 47 J=1,NL
54 DO 47 IK=1,NL2
55 RFS=RESULT(J,IK)
56 R=R*0.529166
57 PCNTRD(J,IK)=PCNTPD(J,IK)*R/RFS
58 R=R*0.529166
59 PRCN(J,IK)=PPCN(J,IK)*R/RFS
60 R=R*0.529166
61 PRRCN(J,IK)=PPRCN(J,IK)*R/RFS
62 R=R*0.529166
63 RRPDM(J,IK)=PPRDM(J,IK)*R/RFS
64 RESULT(J,IK)=RFS*RFS
65 CONTINUE
66 PRINT 107, TITLE
67 NL1S=1$NL1F=10
68 CONTINUE
69 PRINT 109, (KV(J),J=NL1S,NL1F)
70 DO 49 J=1,NL2
71 K=J-1
72 PRINT 108, K,(RESULT(1K,J),1K=NL1S,NL1F)
73 IF (MOD(J,5).NE.0) GO TO 49
74 PRINT 114
75 CONTINUE
76 PRINT 115
77 IF (NL1F.GE.NL) GO TO 50
78 NL1S=NL1F+1$NL1F=NL1S+2
79 IF (NL1F.LT.NL) GO TO 49
80 NL1F=NL1F+2
81 CONTINUE
82 C           SUMMING FCF
83 DO 51 J=1,NL
84 DO 51 JJ=1,NL2
85 SUMPP(J)=SUMPP(J)+RESULT(J,JJ)
86 DO 52 JJ=1,NL2
87 DO 52 J=1,NL
88 SUMP(JJ)=SUMP(JJ)+RESULT(J,JJ)
89 PRINT 79, TITLE
90 DO 53 J=1,NL
91 JM1=J-1
92 PRINT 110, JM1,SUMPP(J)
93 SUMPP(J)=0.
94 DO 54 JJ=1,NL2
95 JM1=JJ-1
96 PRINT 111, JM1,SUMP(JJ)

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54      SUMD(J,J1=0.  
      PRINT 112, TITLE  
      NL1S=1$NL1F=14  
CONTINUE  
      PRINT 127, (KV(J),J=NL1S,NL1F)  
      DO 55 J=1,NL2  
      K=J-1  
      PRINT 113, K,(RCNTRD(ILK,J),ILK=NL1S,NL1F)  
      IF (MOD(J,5).NE.0) GO TO 56  
      PRINT 114  
CONTINUE  
      PRINT 115  
      IF (NL1F.GE.NL1) GO TO 57  
      NL1S=NL1F+1$NL1F=NL1S+12  
      IF (NL1F.LT.NL1) GO TO 58  
      NL1F=NL1GOTO600?  
57      CONTINUE  
      PRINT 116, TITLE  
      NL1S=1$NL1F=14  
CONTINUE  
      PRINT 127, (KV(J),J=NL1S,NL1F)  
      DO 59 J=1,NL2  
      K=J-1  
      PRINT 113, K,(RCNTRD(ILK,J),ILK=NL1S,NL1F)  
      IF (MOD(J,5).NE.0) GO TO 59  
      PRINT 114  
CONTINUE  
      PRINT 115  
      IF (NL1F.GE.NL1) GO TO 60  
      NL1S=NL1F+1$NL1F=NL1S+12  
      IF (NL1F.LT.NL1) GO TO 58  
      NL1F=NL1GOTO600?  
60      CONTINUE  
      PRINT 117, TITLE  
      NL1S=1$NL1F=14  
61      CONTINUE  
      PRINT 127, (KV(J),J=NL1S,NL1F)  
      DO 62 J=1,NL2  
      K=J-1  
      PRINT 113, K,(PRPCN(ILK,J),ILK=NL1S,NL1F)  
      IF (MOD(J,5).NE.0) GO TO 62  
      PRINT 114  
62      CONTINUE  
      PRINT 115  
      IF (NL1F.GE.NL1) GO TO 63  
      NL1S=NL1F+1$NL1F=NL1S+12  
      IF (NL1F.LT.NL1) GO TO 61  
      NL1F=NL1GOTO655?  
63      CONTINUE  
      PRINT 119, TITLE  
      NL1S=1$NL1F=14  
64      CONTINUE  
      PRINT 127, (KV(J),J=NL1S,NL1F)  
      DO 65 J=1,NL2  
      K=J-1

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      PRINT 113, K, (PDRN(ILK,J), ILK=NL1S,NL1F)          A 441
      IF (MOD(J,5).NE.0) GO TO 65                         A 442
      PRINT 114                                         A 443
      CONTINUE                                         A 444
      PRINT 115                                         A 445
      IF (NL1F.GE.NL1) GO TO 66                         A 446
      NL1S=NL1F+1$NL1F=NL1S+1$                          A 447
      IF (NL1F.LT.NL1) GO TO 64                         A 448
      NL1F=NLSGOT0555                                    A 449
      CONTINUE                                         A 450
      PUNCH 119, TITLEF                                 A 451
      PUNCH 121, NL2, NL                                A 452
      PUNCH 122, ((I,J,RESULT(J,I),J=1,NL1),I=1,NL2)    A 453
      PUNCH 123                                         A 454
      PUNCH 124, ((I,J,RCNTRD(J,I),J=1,NL1),I=1,NL2)    A 455
      PUNCH 125                                         A 456
      PUNCH 126, ((I,J,RRCN(J,I),J=1,NL1),I=1,NL2)     A 457
      PUNCH 127                                         A 458
      PUNCH 128, ((I,J,RRRCN(J,I),J=1,NL1),I=1,NL2)    A 459
      DO 67 1K=1,NL2
      DO 67 J=1,NL1
      RESULT(J,IK)=RCNTRD(J,IK)/PRCN(J,IK)
      RCNTRD(J,IK)=PRCN(J,IK)/RRPCN(J,IK)
      RRCN(J,IK)=PPPCN(J,IK)/PRPPN(J,IK)                A 460
      CONTINUE                                         A 461
      PRINT 129, TITLEF                                 A 462
      NL1S=1$NL1F=14                                     A 463
      CONTINUE                                         A 464
      PRINT 127, (KV(J),J=NL1S,NL1F)                   A 465
      DO 69 J=1,NL2
      K=J-1
      PRINT 129, (RESULT(J,ILK),ILK=NL1S,NL1F)          A 466
      PRINT 130, K,(RCNTRD(J,ILK),ILK=NL1S,NL1F)        A 467
      PRINT 131, (RPCN(J,ILK),ILK=NL1S,NL1F)            A 468
      IF (MOD(J,5).NE.0) GO TO 69                         A 469
      PRINT 114                                         A 470
      CONTINUE                                         A 471
      PRINT 115                                         A 472
      IF (NL1F.GE.NL1) GO TO 70                         A 473
      NL1S=NL1F+1$NL1F=NL1S+1$                          A 474
      IF (NL1F.LT.NL1) GO TO 68                         A 475
      NL1F=NLSGOT0601                                    A 476
      CONTINUE                                         A 477
      GO TO 1                                         A 478
      71  VLK=VLK+1
      IF (VLK-VL1M) 20,72,72                           A 479
      72  PRINT 132, VL1M                               A 480
      GO TO 1                                         A 481
      73  PRINT 132, LL1M,I                            A 482
      GO TO 1                                         A 483
      74  PRINT 6, MDF                                 A 484
      GO TO 1                                         A 485
      75  CALL EXIT
      C

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76 FORMAT (11) A 406
77 FORMAT (A10) A 407
78 FORMAT (RA10) A 408
79 FORMAT (14.2F10.0) A 409
80 FORMAT (2F10.0,14) A 410
81 FORMAT (213) A 411
82 FORMAT (214,10A6) A 412
83 FORMAT (14.5F10.0) A 413
84 FORMAT (214,10A6) A 414
85 FORMAT (RF10.0) A 415
86 FORMAT (414.5F10.0) A 416
87 FORMAT (//14H THE MASSES OF THE TWO ATOMS, BASED ON A6.6H, ARF F A 417
110.6,5H AND F10.6//) A 418
88 FORMAT (//14H THE REDUCED MASS OF THE TWO ATOMS, BASED ON A6.5H, A 419
115 F10.6//) A 420
89 FORMAT (35H THE INPUT POTENTIAL POINTS, R IN A6.15H AND ENERGY IN A 421
1 A6.18H ARE GIVEN BELOW. //1X.5(6X,1H,10X,1HV,4X)//) A 422
90 FORMAT (1XF10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F1 A 423
12.4) A 424
91 FORMAT (47H DISSOCIATION ENERGY IN SAME UNITS AS ABOVE ISF20.8) A 425
92 FORMAT (//14H RMIN = F10.7,0H, RMAX = F10.7,12H, SPACING = F10.7 A 426
1.0H, ALL IN A6.1) A 427
93 FORMAT (//14H THE TRIAL ENERGY LEVELS IN A6.16H ARE GIVEN BELOW. A 428
1//1X.5(5H,LFVFL,3X,6HFENERGY,6X)//(1H 14.1PF16.7+14.F16.7+14 A 429
2,F16.7+14,F16.7)) A 430
94 FORMAT (//14H CONVERGENCE CRITERION IS ERROR LESS THAN E9.2+2XA A 431
14) A 432
95 FORMAT (37H THE POTENTIAL FUNCTION GENERATED IS//1X.5(3X,4HR(A), A 433
1AX,2HV(1/CM)2Y)) A 434
96 FORMAT (1X0PF10.6,1PF12.5,4(0PF10.6,1PF12.5),4X15) A 435
97 FORMAT (1XF10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F10.6,F1 A 436
12.4,4X15) A 437
98 FORMAT (30H SCHR FINDS ENERGY LEVEL G = F11.5,15H 1/CM AND RV = F A 438
111.7,5H 1/CM) A 439
99 FORMAT (28H PROGRAM SUCCESSFUL. (MAXIT REACHED 12,7H TIMES)) A 440
100 FORMAT (23H THE BELOW IS FOR THE A10.6H STATE) A 441
101 FORMAT (54H0VIR, NO. GIVEN ENERGY CALC. ENERGY DIFFERENCE1 A 442
12X,4RH GIVEN DELTA G CALC. DELTA G DIFFERENCE/44X,2RH DIFFERENCE A 443
2E = CALC. - GIVEN//) A 444
102 FORMAT (64X2F15.5) A 445
103 FORMAT (18.2F15.5) A 446
104 FORMAT (20H1 THE BELOW IS FOR THE STATE A10) A 447
105 FORMAT (1H02RX,2HY10, NO.,2X,9HCALC. RV5X,2HFXD, RV //) A 448
106 FORMAT (2RY17,2F15.5) A 449
107 FORMAT (28H1 FRANCK CONDON FACTORS FOR .RA10) A 450
108 FORMAT (13.1X,10(2X,F10.3)) A 451
109 FORMAT (1H .2X,2HV,.,=,4X,10(12.10X)/1X,2HV,/) A 452
110 FORMAT (29H THE SUM OVER ALL V- FOR V--=,13.2H15,F12.8) A 453
111 FORMAT (29H THE SUM OVER ALL V-- FOR V--=,13.2H15,F12.8) A 454
112 FORMAT (27H1 P CENTROIDS FACTORS (ANGSTROMS) FOR .RA10) A 455
113 FORMAT (14.14(7X,F6.4)) A 456
114 FORMAT ('H ') A 457
115 FORMAT ('W //') A 458
116 FORMAT (20H1 P**2 CENTROIDS FOR .RA10) A 459
117 FORMAT (20H1 P**3 CENTROIDS FOR .RA10) A 460

```

118	FORMAT (19H1 R**4 CENTROID FOR,RA10)	A 551
119	FORMAT (RA10)	A 552
120	FORMAT (23H FRANCK CONDON FACTORS)	A 553
121	FORMAT (212)	A 554
122	FORMAT (4(2I3,2X,F12.5))	A 555
123	FORMAT (12H P CENTROIDS)	A 556
124	FORMAT (6(1X,2I2,FR.4))	A 557
125	FORMAT (16H R**2 CENTROIDS)	A 558
126	FORMAT (16H R**3 CENTROIDS)	A 559
127	FORMAT (1HO,3X,3HVV=,3X,14(12,7X)/2X+1HV/)	A 560
128	FORMAT (24H1 RATIO OF CENTROIDS FOR,RA10)	A 561
129	FORMAT (1H,4X,14(2X,F6.4))	A 562
130	FORMAT (1H ,12,4X,14(3Y,F6.4))	A 563
131	FORMAT (1H,8X,14(3X,F6.4))	A 564
132	FORMAT (26H0 SCHR NOT SUCCESSFUL FOR I2,2RHTH TIME, GO TO NEXT DPO 1RLEM.)	A 565
133	FORMAT (28H0 SCHR DID NOT CONVERGE FOR I2,17RHTH TIME WHEN I = 13) END	A 566 A 567 A 568-

```

SUBROUTINE POFIT
COMMON XI(60),VI(60),X0(10000),V(10000),S(10000),ETRIAL(30),QIRA(2
1),QIFN(3),QIFMS(2),ZIFMS(2),ZIRA(2),ZIFN(3),FCALC(30),XPRN(5),BVF(30
2),VPRN(5),DTFRMT(10),DUFMT(10),BVF(30),RESULT(30,30),RCNTRD(30,30)
3,RRCN(30,30),RRRCN(30,30),RRRRN(30,30),KV(30),N(2),NL(2),DE(2),PRF
4MT(10),PNFT(10),DIV(50),SUMPP(30),SUMP(30),TITLE(8),XH,NSTA,MSTA,M
5,XMIN,XMAX,INSC,MREG,MUSED,NI,NS,MAXIT,FACH,ZMU,IKON,EPS,IPSIQ,SCH
6P,SU(10000)
DIMENSION Z(60),AX(60),RY(60),CX(60),DX(60)
YMAXT=XMAY
XMINT=XMIN
C CHECK FOR EXTRAPOLATION AT SMALL R.
IF (XMINT-XI(1)) .LT. 2
1 XMAX=XI(1)
INSC=1
NLL=N(IKON)
CALL XTRAP (XI,VI,Z,NLL,X0,V,M,XH,XMIN,XMAX,INSC,FACH,MREG,DE(IKON))
MT=M
YMIN=X0(MT)+VH
MREG=M+1
C PREPARE TO INTERPOLATE.
2 M=0
XMAX=XMAXT
IF (XMAX-XI(NLL)) .LT. 4,4,3
3 XMAX=XI(NLL)
CALL SPLXYZ (XI,VI,Z,NLL,AX,RY,CX,DX)
MEND=MREG+INT((XMAX-XMIN)/XH)
Y00=XMIN
DO 5 IT=MREG,MEND
CALL SPNXYZ (XI,VI,Z,NLL,Y00,VO)
VI(IT)=VO
Y0(IT)=Y00
5 X00=Y00+XH
C CHECK FOR EXTRAPOLATION AT LARGE R.
IF (YMAXT-XMAX) .LT. 2,7,6
6 MREG=MEND+1
XMIN=X0(MREG-1)+XH
XMAX=XMAXT
INSC=2
CALL XTRAP (XI,VI,NLL,X0,V,M,YH,XMIN,XMAX,INSC,FACH,MREG,DE(IKON))
INSC=2
7 YMIN=XMIN
M=MREG-1
RETURN
END

```

```

SUBROUTINE SPLXYZ (Y,Y,Z,N,A,B,C,DY)
DIMENSION Y(1), Z(1), T(1)
DIMENSION A(1), B(1), C(1), DY(1)
DATA D6/01715E2E252525252525252/
DATA D3/01716E25252525252525252/
NP=N-1
NQ=N-2
DO 2 K=1,NP
DX(K)=Y(K+1)-Y(K)
IF (DX(K)) 1+1+2
1 PRINT 6, Y(K), Y(K+1), DY(K), T
STOP 301
2 CONTINUE
A(1)=-DY(1)
C(1)=-1./DX(2)
B(1)=1./DX(1)-C(1)
Z(1)=0.
DYX=(Y(2)-Y(1))/DX(1)
DO 3 K=2,NP
KK=K-1
A(K)=DY(KK)*D6
B(K)=(DY(K)+DY(KK))*D3
C(K)=DY(K)*D6
DYXP=DYX
DYX=(Y(K+1)-Y(K))/DX(K)
Z(K)=DYX-DYXP
3 CONTINUE
AA=-1./DX(NQ)
CC=-1./DY(NP)
BB=(AA+CC)
A(N)=AA*B(NP)-A(NP)*BB
B(N)=AA*C(NP)-A(NP)*CC
Z(N)=AA*Z(NP)
XF=A(2)*A(1)
B(2)=B(2)-XF*B(1)
C(2)=C(2)-XF*C(1)
DO 4 K=2,NP
KK=K+1
YF=A(KK)/B(K)
B(KK)=B(KK)-XF*C(K)
Z(KK)=Z(KK)-XF*Z(K)
4 CONTINUE
Z(N)=Z(N)/B(N)
DO 5 K=1,NQ
KK=N-K
Z(KK)=(Z(KK)-Z(KK+1)*C(KK))/B(KK)
CONTINUE
Z(1)=-(Z(2)*B(1)+Z(3)*C(1))*A(1)
RETURN
6 FORMAT (1H1,1X,3E25.15,115)
END

```

```

1      SUBROUTINE SRNXYZ (X,Y,Z,N,IUX,ILY)
2      DIMENSION X(1), Y(1), Z(1)
3      DATA Y6A/01715E252E257E252E252E/
4      IF (IUX-X(1)) .LT. 0.
5      PRINT 12, IUX,Y(1),Y(N),ILY
6      STOP 311
7      ILY=Y(1)
8      RETURN
9      IF ((IY-Y(N)) .LE. 4.0)
10     ILY=Y(N)
11     RETURN
12     SH=N
13     SL=1.
14     I=(SH+SL)*E
15     IF ((IUX-X(1)) .GE. 1.0)
16     SH=I
17     IF (SH-SL-1.) .GT. 12.0
18     STOP 312
19     SL=I
20     GO TO 9
21     ILY=Y(1)
22     RETURN
23     MA=SL
24     MA=SH
25     YA=X(MA)-X(")
26     YAA=YA*YA
27     XAR=1./XA
28     YR=Y(MA)-ILY
29     YRA=YR*YR
30     YRR=YR*(YRA-YAA)
31     YC=ILY-Y(")
32     YCA=YC*YC
33     YCC=YC*(YCA-YAA)
34     IY=((Z(")*YRR+Z(MA)*YCC)+Y(MA)*YC+Y(")*XR)*XAR
35     RETURN
36
37     FORMAT (1H1,1X,2E25.15,115)
38
39     END

```

```

SUBROUTINE XTRAP (X1,Y1,N,X0,V,M,XH,XMIN,YMAX,INSC,FACH,MREG,DF)      F   1
DIMENSION XI(1), YI(1), X0(1), V(1), EN(2), XL(6), YL(6), SIGH(1),    F   2
1 ANS(4)                                                               F   3
C   V=C1*B**((A*LOG(P)+B)                                         F   4
C   DF(X)=C1*X**((A*ALOG(X)+B)                                       F   5
C   DF1(X)=DF-DF(X)                                                 F   6
C   IF (INSC.GT.1) GO TO 2                                           F   7
C   INITIALIZING SECTION FOR INNER BRANCH OF POTENTIAL               F   8
M=XFIXF((YMAX-XMIN)/YH)+1                                         F   9
MP=1                                                               F  10
IST=1                                                               F  11
IFIN=M                                                               F  12
C   LEAST SQUARES PARAMETERS                                         F  13
ILS=1ST,LF=6                                                       F  14
DO 1 I=ILS,LF
XL(I)=ALOG(XI(I))                                                 F  15
1 YL(I)=ALOG(YI(I))                                                 F  16
MPTS=6,NODER=2,NINT=1                                             F  17
SIGH(1)=XL(MPTS)
CALL LSOPRT (XL,YL,NINT,NORDER,MPTS,SIGH,ANS)                   F  18
A=0.
B=ANS(2)
GO TO 4
C   INITIALIZING SECTION FOR OUTER BRANCH OF POTENTIAL             F  24
2 M=XFIXF((YMAX-XMIN)/YH)+1                                         F  25
IFIN=MREG+M-1                                                       F  26
IST=MREG
MP=N                                                               F  27
C   SET UP LEAST SQUARES PARAMETERS                                     F  28
ILS=N-5,LF=N                                                       F  29
C   FINDING A, B BY LEAST SQUARES METHOD FROM LAST 6 POINTS OF POTENT F  30
J=1                                                               F  31
DO 3 I=ILS,LF
XL(J)=ALOG(XI(I))                                                 F  32
YL(J)=ALOG(YI(I))                                                 F  33
3 J=J+1
MPTS=6
NORDER=2
NINT=1
SIGH(1)=XL(MPTS)
CALL LSOPRT (XL,YL,NINT,NORDER,MPTS,SIGH,ANS)                   F  34
A=0.
B=ANS(2)
C=ANS(1) BUT NOT USED
CONTINUE
D1=B*A*ALOG(XI(MP))+520166)*B
D1=A*ALOG(YI(MP))+B
IF (INSC.GT.1) GO TO 5
C1=YI(MP)/XI(MP)**D1
GO TO 6
5 C1=(DF-VI(MP))/XI(MP)**D1
CONTINUE
DO 9 I=IST,IFIN
X0(I)=FLOAT(I-IST)*XH+XMIN
IF (INSC.GT.1) GO TO 7

```

```

V(1)=PF(Y0(1))
F 56
GO TO 9
E 57
V(1)=PF1(Y0(1))
F 58
CONTINUE
F 59
CONTINUE
F 60
PRINT VARIABLE
F 61
C1=C1*FACT#0.529166**D1D
F 62
FN(2)=SHRIGHT
F 63
FN(1)=SHLEFT
F 64
PRINT 10, FN(INSC)
F 65
PRINT 11, A,B,C1,D1D
F 66
OPTION
F 67
E 68
10 FORMAT (//4H THE PARAMETERS USED TO EXTRAPOLATE THE AR,46H BRANC E 69
1H OF THE POTENTIAL CURVE ARE AS FOLLOWS /)
E 70
11 FORMAT (3H A=F10.3,3H B=F10.3,4H C1=F10.3,4H D1=F10.3,32H MMFRF V= F 71
1C1*X**D1, D1=A*LOG(V)+B//)
E 72
END F 73-

```

```

SUBROUTINE SCHRO (KV,F0) F 1
C NOTE COMMON NAMES HAVE BEEN CHANGED TO MAKE BLOCK COMPARABLE F 2
C WITH THIS SUBROUTINE F 3
COMMON X1(60),Y1(60),YO(10000),V(10000),G(10000),FTRIAL(30),OIRAI(2 F 4
11,OIEN(3),OIMS(2),ZIMS(2),ZIRAI(2),ZIFN(3),FCALC(30),XPRN(5),BVF(30 F 5
21),VPRN(5),DTFRMT(10),DUFMT(10),BVF(30),RESULT(30,30),RCNTRD(30,30) F 6
3,RRCN(30,30),RRRCN(30,30),RRRRN(30,30),TV(30),L(2),NN(2),DD(2),PRF F 7
4MT(10),PNFT(10),DIV(50),SUMPP(30),SUMP(30),TITLE(8),XH,NSTA,MSTA,N F 8
5,XMIN,XMAX,INSC,MREG,MUSED,NI,NS,MAXIT,FACM,ZMU,IKON,EPS,IPSIQ,SCH F 9
6P,SU(10000) F 10
DIMENSION Y(3), R(10000) F 11
EQUIVALENCE (R,Y0), (YMIN,PMINI), (YMAX,RMAX) F 12
SCHR V PRINTS EVERY IPSIQ'TH POINT OF THE WAVE FUNCTIONS. F 13
RADIAL SOLUTION TO SCHRÖDINGER EQUATION SUBROUTINE F 14
USE UNITS SUCH THAT SCHR EON IS -PSI2 + (F-V)PSI = 0 F 15
NI=1, PRINT ITERATIONS F 16
NI=OTHERWISE, DONT PRINT F 17
NS=1, PRINT SOLUTIONS WITH EACH ENERGY LEVEL F 18
NS=32, PRINT ENERGY LEVELS ONLY F 19
NS=OTHERWISE, DONT PRINT F 20
IF (NI-1) 2,1,2 F 21
1 FPRIN=F0*FACM F 22
PRINT 42, KV,FPRIN F 23
PRINT 43 F 24
2 CONTINUE F 25
H=(RMAX-RMIN)/FLOAT(N-1) F 26
H2=H**2 F 27
HV=H2/12. F 28
F=F0 F 29
TEST=-1. F 30
DF=0. F 31
C START ITER LOOP F 32
C DO 22 IT=1,MAXIT F 33
C .....START INWARD INTEGRATION F 34
D(N)=1,F=20 F 35
GN=V(N)-F F 36
GI=V(N-1)-F F 37
C .....TEST IF F TOO HIGH F 38
IF (GI) 3,4,4 F 39
3 PRINT 44 F 40
SCHR=2. F 41
GO TO 41 F 42
4 D(N-1)=D(N)*EXP(-(RMAX*G0)-(RMAX-H)*G0) F 43
Y=(1.-HV*GN)*D(N) F 44
Y(2)=(1.-HV*G1)*D(N-1) F 45
C .....INTEGRATE F 46
M=N-2 F 47
5 Y(2)=Y(2)+((Y(2)-Y)+H2*G1)*D(M+1) F 48
G1=Y(M)-F F 49
D(M)=Y(2)/(1.-HV*G1) F 50
C .....OVERFLOW F 51
M1=M+1 F 52
DM=D(M) F 53

```

```

      DO 6 J=M1,N
      P(J)=P(J)/DM
      Y=Y/DM
      V(2)=V(2)/DM
      V(3)=V(3)/DM
      GT=V(N+1)-F
      GO TO 5
C     *****TEST FOR CROSSING PT.
      IF (ABSF(P(M))-ABSF(P(M+1))) .GT. 0.007
      IF (M-2) 0,0,8
      Y=Y(2)
      V(2)=Y(2)
      M=M-1
      GO TO 5
C
      DM=P(M)
      M$AVF=M
      V1N=Y(2)/DM
      DO 10 J=M,N
      P(J)=P(J)/DM
C     *****START OUTWARD INTEGRATION
      P(1)=1.E-20
      Y=0.
      GT=V-F
      V(2)=(1.0-HV*GT)*P
      DO 13 I=2,M
      Y(3)=Y(2)+((V(2)-Y)+H2*GI*P(I-1))
      GI=V(I)-F
      P(I)=Y(3)/(1.0-HV*GI)
      I1=I-1
      DM=P(I1)
      DO 12 J=1,I1
      P(J)=P(J)/DM
      Y=Y/DM
      V(2)=Y(2)/DM
      V(3)=Y(3)/DM
      GI=V(I1)-F
      GO TO 13
C
      Y=Y(2)
      V(2)=Y(2)
C     *****FINISHED OUTWARD INTEGRATION
      DM=P(M)
      IF (DM) 14,17,14
      YOUT=Y/DM
      YM=Y(2)/DM
      DO 15 J=1,M
      P(J)=P(J)/DM
C     *****CORRECTION
      DF=0.

```

```

16 DO 16 J=1,N F 111
    DF=DF-P(J)**2 F 112
    F=(-YOUT-Y(N+2)*Y(N))/H2+(V(N)-F) F 113
    POLD=DF F 114
17 F=9.000000E+20 F 115
    DF=-F F 116
    DF=ARSF(1.0001*F) F 117
    GO TO 18 F 118
    DF=-F/DF F 119
18 IF (N1-1) 20,19,20 F 120
19 EPRINT=F*FACH F 121
    DPRINT=DF*FACH F 122
    PRINT 45, IT,EPRINT,F,DF,DPRINT,MSAVE F 123
20 FOLD=F F 124
    F=F+DF F 125
    TEST=MAX1F(ARSF(POLD)-ARSF(DF),TEST) F 126
    IF (TEST) 22,21,21 F 127
21 IF (ARSF(F-FOLD)-ARSF(FPS)) 23,23,22 F 128
22 CONTINUE F 129
    SCHR=1. F 130
    GO TO 24 F 131
C     .....CONVERGED-COUNT NODES F 132
23 SCHR=0. F 133
24 KV=0 F 134
    NL=N-2 F 135
    DO 34 J=3,NL F 136
    IF (P(J)) 26,25,25 F 137
25 IF (P(J-1)) 27,24,24 F 138
26 IF (P(J-1)) 34,31,20 F 139
C     POS. NODE F 140
27 IF (P(J+1)) 34,28,28 F 141
28 IF (P(J-2)) 22,24,24 F 142
C     NEG. NODE F 143
29 IF (P(J+1)) 30,34,24 F 144
30 IF (P(J-2)) 34,33,33 F 145
C     FALSE NODE DUE TO UNDERFLOW F 146
31 IF (P(J+1)) 32,34,34 F 147
32 IF (P(J-2)) 34,34,33 F 148
33 KV=KV+1 F 149
34 CONTINUE F 150
C     .....NORMALIZE F 151
    SN=50*TE(-H*DF) F 152
    DO 35 J=1,N F 153
    C(J)=P(J)/SN F 154
C     .....PRINT SOLUTION F 155
    PER*FACH F 156
    IF (NS-1) 38,36,38 F 157
35 TPSIA=TPSI10*300 F 158
    TPSIB=TPSI10*40 F 159
    TPSIC=TPSI10*250 F 160
    TPSID=TPSI10*50 F 161
    DO 37 JF=1,N,1PSIA F 162
    DPRINT 46, KV,M F 163
    PRINT 46, KV,F F 164
    JI=EXITMODE(JF+1PSI10,N)

```

```

00 37 J=JF+JL+IPS10          F 165
JL=XMINCF(L+IPS10,0)        F 166
PRINT 47, (I+5)(I)+I=J+JL+IPS10   F 167
CONTINUE                      F 168
38 EOF                         F 169
IF (MS-33) 40,30,40           F 170
PRINT 48, KV*F                F 171
40 CONTINUE                     F 172
41 RETURN                       F 173
C
42 DORMUT (4701SLP- SOLUTION OF R1491L S3AR. EQUATION FOR V=13.5X.7H F 174
42 FORMAT (47HISCHR- SOLUTION OF RADIAL SCHR. EQUATION FOR V=13.5X.7H F 175
1FTRIAL=1PF15.7,9H (1/CM))    F 176
43 FORMAT (7DH0) 1TFR          F(F)      DF(F)  F 177
1  DF(F)  )                   F 178
44 FORMAT (50H DIFFERENCE EQUATION SOLUTION TECHNIQUE FAILS  )       F 179
45 FORMAT (1H0)4.2X,1P4F16.7,5X,29H THF CROSSING PT. OCCURS AT 14) F 180
46 FORMAT (47HISCHR- SOLUTION OF RADIAL SCHR. EQUATION FOR V=13.7H F 181
1  F=1PF15.7/2CH0 1  S(I)  S(2H) 1  S(I)  )       F 182
47 FORMAT (6(1E,1PF15.7))      F 183
48 FORMAT (50H0 SOLUTION OF RADIAL SCHRODINGER EQUATION FOR V = 13.7H F 184
1  F = 1PF15.7)              F 185
END                          F 186-

```

```
C      SUBROUTINE SIMP (S,SS,N,H,RESULT)
C      INTEGRATION OF A PRODUCT SAY SIMPSONS RULE.
C      DIMENSION S(2000), SS(2000)
C      SUM=0.0
1      DO 1 J=2,N,2
      SUM=SUM+2.0*S(J)*SS(J)+4.0*S(J-1)*SS(J-1)
      RESULT=SUM*H/3.0
      RETURN
      END
```

G	1
G	2
G	3
G	4
G	5
G	6
G	7
G	8
G	9
G	0.

APPENDIX III

TABLE OF R-CENTROIDS

Table 95

Table 95 (cont'd)

100-250 (4/21)

Table 96

112/111 C52 NO 2695 SICERNEC-2

Table 96 (cont'd)

(CN 2EJ (3/21)

γ	$\nu\nu$	$\Delta\nu$	11	12	13	14	15	16	17	18
1	1.673-	1.317-	1.0491-	1.324-	1.367-	1.295-	1.194-	1.314-	1.243-	1.243-
4	1.241-	1.121-	1.317-	1.272-	1.553-	1.335-	1.51-	1.339-	1.197-	1.197-
2	941-1	2.65-	1.195-	1.593-	1.271-	1.592-	1.413-	1.267-	1.635-	1.635-
3	616-	3.996-	1.243-	1.413-	1.477-	1.262-	1.271-	1.516-	1.306-	1.306-
4	1.692-	1.717-	2.517-	1.224-	1.142-	1.842-	1.259-	1.165-	1.992-	1.992-
5	1.551-	1.669-	1.754-	2.322-	1.191-	1.220-	1.261-	1.193-	1.193-	1.193-
2	1.431-	1.367-	1.670-	2.795-	1.74-	1.65-	1.196-	8.729-	1.216-	1.216-
7	1.421-	1.421-	1.575-	1.694-	1.415-	2.255-	1.161-	1.234-	2.249-	2.249-
4	1.394-	1.431-	1.439-	1.593-	1.533-	1.324-	2.242-	1.311-	1.305-	1.305-
3	1.355-	1.443-	1.443-	1.532-	1.532-	1.762-	1.636-	2.161-	2.203-	2.203-
12	2.121-	1.317-	9.939-	1.451-	1.516-	1.606-	1.711-	1.847-	2.176-	2.176-
11	1.230-	1.213-	1.328-	1.301-	1.452-	1.525-	1.619-	1.719-	1.860-	1.860-
12	1.156-	1.250-	1.252-	1.343-	1.343-	1.475-	1.534-	1.618-	1.729-	1.729-
13	1.136-	1.199-	1.270-	1.270-	1.353-	1.371-	1.496-	1.544-	1.627-	1.627-
14	1.161-	1.154-	1.213-	1.312-	1.243-	1.369-	1.396-	1.508-	1.554-	1.554-
15	1.211-	1.421-	1.107-	1.221-	4.434-	1.296-	1.392-	1.399-	1.536-	1.536-
13	1.641-	1.123-	1.13-	1.179-	1.214-	1.199-	1.308-	1.416-	1.416-	1.416-
17	1.125-	1.936-	1.140-	1.133-	1.139-	1.220-	1.234-	1.321-	1.716-	1.716-
14	1.031-	1.303-	1.093-	1.195-	1.149-	1.199-	1.275-	1.255-	1.335-	1.335-

Table 97

TABLE 97
FOR COMPUTATION OF

<i>J</i>	<i>N</i>	2	3	4	5	6	7	8	9
1	1.1 2-1	1.0 12 2-1	9. 715-1	9. 0-2-1	9. 0-2-1	3. 0-2-1	1. 227-1	1. 167-0	3. 379-0
2	1.2 1-1	1.0 17 3-1	1.0 57-1	1.0 96 3-1	1.0 157-1	1.0 341-1	7. 0 326-1	9. 0 137-1	1.0 316-0
3	1.3 0-1	1.0 21 2-1	1.0 147-1	1.0 159-1	1.0 942-1	1.0 15d-1	1.0 409-1	7. 0 449-1	1.0 356-1
4	1.4 0-1	1.0 25 2-1	1.0 55-1	1.0 139-1	1.0 038-1	1.0 954-1	1.0 149-1	8. 0 432-1	7. 0 315-1
5	1.5 2-1	1.0 29 2-1	1.0 55-1	1.0 139-1	1.0 038-1	1.0 954-1	1.0 149-1	8. 0 432-1	7. 0 315-1
6	1.6 3-1	1.0 316-1	1.0 522-1	1.0 315-1	1.0 212-0	1.0 154-0	1.0 171-1	9. 0 150-1	1.0 503-1
7	1.7 3-1	1.0 316-1	1.0 522-1	1.0 315-1	1.0 212-0	1.0 154-0	1.0 171-1	9. 0 150-1	1.0 503-1
8	1.8 4-1	1.0 224-1	1.0 553-1	1.0 590-1	1.0 328-1	1.0 226-1	1.0 146-1	1. 0 111-1	1. 0 554-1
9	1.9 4-1	1.0 224-1	1.0 553-1	1.0 590-1	1.0 328-1	1.0 226-1	1.0 146-1	1. 0 111-1	1. 0 554-1
10	2.0 4-1	1.0 377-1	1.0 553-1	1.0 659-1	1.0 173-1	1.0 342-1	1.0 242-1	1. 0 129-1	1. 0 119-1
11	2.1 4-1	1.0 377-1	1.0 553-1	1.0 659-1	1.0 173-1	1.0 342-1	1.0 242-1	1. 0 129-1	1. 0 119-1
12	2.2 4-1	1.0 295-1	1.0 295-1	1.0 462-1	1.0 173-1	1.0 253-0	1.0 253-0	9. 0 973-1	1. 0 132-1
13	2.3 4-1	1.0 295-1	1.0 295-1	1.0 462-1	1.0 173-1	1.0 253-0	1.0 253-0	9. 0 973-1	1. 0 132-1
14	2.4 4-1	1.0 172-1	1.0 672-1	1.0 339-1	1.0 141-1	2. 0 125-0	1. 0 259-1	1. 0 276-1	9. 0 406-1
15	2.5 4-1	1.0 172-1	1.0 672-1	1.0 339-1	1.0 141-1	2. 0 125-0	1. 0 259-1	1. 0 276-1	9. 0 406-1
16	2.6 4-1	1.0 225-1	1.0 174-1	1.0 913-1	1.0 525-0	1.0 363-0	1.0 381-4	7. 0 9d0-1	1. 0 434-1
17	2.7 4-1	1.0 225-1	1.0 174-1	1.0 913-1	1.0 525-0	1.0 363-0	1.0 381-4	7. 0 9d0-1	1. 0 434-1
18	2.8 4-1	1.0 266-0	1.0 147-1	1.0 131-1	1.0 142-1	2. 0 411-1	1. 0 447-1	6. 0 374-1	1. 0 456-1
19	2.9 4-1	1.0 266-0	1.0 147-1	1.0 131-1	1.0 142-1	2. 0 411-1	1. 0 447-1	6. 0 374-1	1. 0 456-1
20	3.0 4-1	1.0 125-1	1.0 531-1	9. 0 949-1	1.0 175-0	1.0 2+1-1	1.0 130-1	1.0 089-1	1.0 362-0
21	3.1 4-1	1.0 125-1	1.0 531-1	9. 0 949-1	1.0 175-0	1.0 2+1-1	1.0 130-1	1.0 089-1	1.0 362-0
22	3.2 4-1	1.0 306-1	1.0 177-1	1.0 316-0	1.0 165-0	1.0 265-0	1.0 255-0	1.0 210-0	1. 0 222-1
23	3.3 4-1	1.0 306-1	1.0 177-1	1.0 316-0	1.0 165-0	1.0 265-0	1.0 255-0	1.0 210-0	1. 0 222-1
24	3.4 4-1	1.0 7 7-1	1.0 132-1	1.0 131-1	1.0 237-0	1.0 237-0	1.0 259-0	1.0 181-1	1. 0 413-0
25	3.5 4-1	1.0 7 7-1	1.0 132-1	1.0 131-1	1.0 237-0	1.0 237-0	1.0 259-0	1.0 181-1	1. 0 413-0
26	3.6 4-1	1.0 446-1	1.0 225-1	1.0 174-1	1.0 913-1	1.0 525-0	1.0 363-0	1.0 381-4	7. 0 9d0-1
27	3.7 4-1	1.0 446-1	1.0 225-1	1.0 174-1	1.0 913-1	1.0 525-0	1.0 363-0	1.0 381-4	7. 0 9d0-1
28	3.8 4-1	1.0 246-0	1.0 147-1	1.0 131-1	1.0 142-1	2. 0 411-1	1. 0 447-1	6. 0 374-1	1. 0 456-1
29	3.9 4-1	1.0 246-0	1.0 147-1	1.0 131-1	1.0 142-1	2. 0 411-1	1. 0 447-1	6. 0 374-1	1. 0 456-1
30	4.0 4-1	1.0 125-1	1.0 531-1	9. 0 949-1	1.0 175-0	1.0 2+1-1	1.0 130-1	1.0 089-1	1.0 362-0
31	4.1 4-1	1.0 125-1	1.0 531-1	9. 0 949-1	1.0 175-0	1.0 2+1-1	1.0 130-1	1.0 089-1	1.0 362-0
32	4.2 4-1	1.0 121-1	1.0 121-1	1.0 193-0	1.0 193-0	1.0 427-1	1. 0 311-0	1. 0 487-1	1. 0 274-1
33	4.3 4-1	1.0 121-1	1.0 121-1	1.0 193-0	1.0 193-0	1.0 427-1	1. 0 311-0	1. 0 487-1	1. 0 274-1
34	4.4 4-1	1.0 2417-1	2. 0 417-1	1.0 077-1	1.0 126-1	1.0 126-1	2. 0 117-1	1. 0 216-1	1. 0 379-1
35	4.5 4-1	1.0 2417-1	2. 0 417-1	1.0 077-1	1.0 126-1	1.0 126-1	2. 0 117-1	1. 0 216-1	1. 0 379-1
36	4.6 4-1	1.0 353-1	1.0 353-1	1.0 771-1	1.0 771-1	1.0 2+1-0	1. 0 543-0	1. 0 396-1	1. 0 549-0
37	4.7 4-1	1.0 353-1	1.0 353-1	1.0 771-1	1.0 771-1	1.0 2+1-0	1. 0 543-0	1. 0 396-1	1. 0 549-0
38	4.8 4-1	1.0 2+1-1	1.0 2+1-1	2. 0 62-1	2. 0 62-1	1.0 113-1	3. 0 353-1	1. 0 016-1	1. 0 495-0
39	4.9 4-1	1.0 2+1-1	1.0 2+1-1	2. 0 62-1	2. 0 62-1	1.0 113-1	3. 0 353-1	1. 0 016-1	1. 0 495-0

Table 97 (cont'd)

(CON'VOLUTED)

	V	11	12	13	14	15	16	17	18
1	1.0237-1	1.01164-3	8.0346-1	9.0412-1	1.0216-4	9.026-1	1.0357-4	1.0110-3	
2	1.0241-1	1.0251-3	1.0129-1	1.0123-2	1.0341-3	1.0141-3	1.049-3	9.009-1	9.025-1
3	1.0244-1	1.0255-3	1.0239-1	1.0164-5	1.0146-1	1.0142-1	1.0128-0	1.0131-3	1.033-1
4	1.0246-1	1.031-1	1.0179-1	1.0126-6	1.0439-3	3.0336-7	9.0522-1	1.0554-0	1.032-3
5	1.0256-1	7.0773-1	1.0325-3	1.0134-7	1.0159-1	1.0159-1	1.0758-0	6.035-1	1.033-3
6	1.0266-1	9.0745-1	7.0532-1	1.0305-6	1.0123-3	1.0353-0	7.0491-1	9.0309-1	6.0179-1
7	1.0522-1	7.0539-1	4.0596-1	4.0145-6	1.0299-3	1.0574-3	1.0045-0	9.006-1	3.0314-1
8	1.0935-1	9.0468-1	7.0427-1	4.0373-1	3.0313-3	1.0296-3	1.074-0	9.069-1	9.0718-1
9	1.0349-1	1.0745-1	6.055-1	7.0211-1	4.0313-1	3.0533-6	1.034-0	1.0190-3	9.0498-1
10	3.064-1	1.0074-5	8.0405-1	8.0613-1	3.0999-1	6.0963-1	3.0838-0	1.0332-9	1.0116-3
11	1.0344-1	2.0933-1	1.0169-3	7.0793-1	4.0083-3	6.0261-1	5.0560-1	5.0328-0	1.0400-0
12	1.0474-1	1.0316-0	3.0371-1	1.0151-6	6.0512-1	9.0462-1	4.0935-1	7.0033-1	9.0706-1
13	1.0244-1	1.0540-0	1.0326-3	1.0271-3	1.0213-3	3.0135-1	1.038-0	9.0624-1	6.0112-1
14	1.0754-1	1.0230-1	1.0218-1	1.0371-6	1.0219-0	1.0260-0	1.0256-0	1.0150-0	1.0073-0
15	1.0325-1	2.0933-0	1.0336-7	2.0771-6	1.0339-6	3.0568-6	1.0319-0	5.0662-1	1.0257-1
16	3.0276-1	1.0416-1	5.0394-1	1.0397-6	4.0657-1	1.0320-0	2.0520-0	1.0369-1	2.0610-0
17	1.0742-1	1.0446-3	1.0516-1	1.0172-3	1.0442-1	1.0179-1	1.0238-0	2.0399-1	1.0400-0
18	1.0369-1	2.0550-0	1.0246-1	1.0722-0	1.0233-1	1.0524-1	1.0292-0	1.0247-1	2.0377-1
19	4.0115-1	1.0513-1	2.0599-1	1.0254-6	3.0453-3	1.0319-1	1.0745-0	1.0298-1	1.0131-3

Table 98

卷之三

Table 98 (cont'd)

(CO 474 +)

<i>N</i>	13	14	15	16	17	18	19	20	21	22	23	24
V	1.374-6	1.531-6	1.244-0	8.955-1	1.325-0	1.126-0	9.412-1	1.447-0	1.242-0	2.311-1	8.869-1	1.176-0
1	1.364-6	1.546-7	1.264-0	1.765-0	1.115-0	1.333-0	1.027-1	1.177-1	1.120-0	1.126-0	1.235-0	1.224-0
2	1.525-1	1.346-1	1.346-0	3.363-0	1.129-0	1.411-0	1.345-0	1.259-0	1.416-0	1.252-0	2.316-0	1.636-0
3	1.511-1	1.538-4	1.293-0	1.702-0	1.463-1	1.510-0	1.523-0	1.453-0	1.763-0	1.355-0	1.196-0	1.437-0
4	1.487-0	1.214-0	1.533-0	1.593-0	1.639-0	1.649-0	1.549-0	1.732-0	1.359-0	1.598-0	1.464-0	1.437-0
5	1.466-7	1.416-7	1.229-2	1.581-0	1.593-0	1.022-0	1.642-0	1.636-0	2.160-0	1.322-0	1.431-0	1.091-0
6	1.445-7	1.475-6	1.535-0	1.536-0	1.557-0	1.539-0	1.628-0	1.659-0	1.719-0	2.006-0	1.997-0	1.522-0
7	1.426-7	1.455-7	1.416-0	1.513-0	1.564-0	1.575-0	1.606-0	1.611-0	1.677-0	1.717-0	1.702-0	1.736-0
8	1.402-7	1.429-0	1.405-0	1.435-0	1.522-0	1.553-0	1.524-0	1.616-0	1.649-0	1.693-0	1.711-0	1.754-0
9	1.388-7	1.413-0	1.441-0	1.446-0	1.513-0	1.532-0	1.532-0	1.562-0	1.593-0	1.624-0	1.698-0	1.725-0
10	1.364-7	1.316-4	1.424-0	1.422-0	1.477-0	1.517-0	1.542-0	1.571-0	1.612-0	1.633-0	1.665-0	1.710-0
11	1.335-7	1.376-0	1.433-0	1.433-0	1.462-0	1.499-0	1.475-0	1.553-0	1.591-0	1.611-0	1.643-0	1.675-0
12	1.327-8	1.356-1	1.390-0	1.415-0	1.439-0	1.475-0	1.511-0	1.526-0	1.569-0	1.592-0	1.622-0	1.653-0
13	1.313-8	1.352-0	1.359-0	1.331-0	1.426-0	1.473-0	1.519-0	1.513-0	1.537-0	1.555-0	1.615-0	1.633-0
14	1.287-6	1.326-1	1.347-0	1.342-0	1.417-0	1.463-0	1.465-0	1.498-0	1.527-0	1.550-0	1.575-0	1.636-0
15	1.287-6	1.358-0	1.342-0	1.364-0	1.399-0	1.420-0	1.444-0	1.477-0	1.503-0	1.475-0	1.563-0	1.597-0
16	1.274-6	1.253-0	1.323-0	1.333-0	1.377-0	1.401-0	1.434-0	1.457-0	1.499-0	1.516-0	1.539-0	1.591-0
17	1.256-6	1.256-0	1.256-0	1.333-0	1.367-0	1.392-0	1.416-0	1.453-0	1.471-0	1.496-0	1.530-0	1.553-0
18	1.246-6	1.271-0	1.104-0	1.322-0	1.210-0	1.374-0	1.395-0	1.430-0	1.452-0	1.487-0	1.510-0	1.625-0
19	1.232-6	1.227-0	1.237-0	1.337-0	1.340-0	1.358-0	1.390-0	1.415-0	1.449-0	1.469-0	1.439-0	1.524-0
20	1.223-6	1.244-0	1.233-0	1.231-0	1.579-0	1.231-0	1.342-0	1.602-0	1.399-0	1.446-0	1.308-0	5.496-0

Table 99

ψ -C₄₄(201)S F12 (N(2) 1ST. +)

ψ_1	ψ_2	ψ_3	ψ_4	ψ_5	ψ_6
1 1.234-4	1.216-4	1.113-4	1.122-4	1.125-4	1.103-4
2 1.231-4	1.317-4	2.227-4	1.192-4	1.151-4	1.133-4
2 1.347-4	1.319-4	1.227-4	1.249-4	1.213-4	1.171-4
3 1.043-4	1.357-4	1.323-4	1.271-4	1.139-4	1.219-4
4 1.465-4	1.412-4	1.367-4	1.367-4	1.243-4	1.236-4
5 1.547-4	1.477-4	1.421-4	1.373-4	1.247-4	1.296-4
6 1.647-4	1.225-4	1.445-4	1.431-4	1.336-4	1.322-4
7 1.734-4	1.657-4	1.564-4	1.495-4	1.441-4	1.477-4
8 2.241-4	1.744-4	1.656-4	1.574-4	1.515-4	1.452-4
9 1.142-4	2.033-4	1.739-4	1.675-4	1.534-4	1.515-4
10 1.954-4	1.164-4	2.042-4	1.919-4	1.645-4	1.593-4
11 1.644-4	1.054-4	1.369-4	2.069-4	1.931-4	1.696-4
12 1.270-4	1.544-4	1.245-4	2.059-4	2.031-4	1.969-4
13 1.205-4	1.144-4	1.556-4	1.336-4	3.034-4	2.099-4
14 3.517-4	1.121-4	1.296-4	1.722-4	1.523-4	5.097-4
15 1.355-4	1.233-4	9.213-4	1.316-4	3.050-4	1.397-4
16 1.316-4	1.533-4	5.491-4	1.219-4	1.179-4	1.069-4
17 1.331-4	1.355-4	1.331-4	2.195-4	1.232-4	9.941-4

Table 99 (cont'd)

(V(2) ISR. +)

ν	JW	J	δ	α	β_J	β_L	β_2	β_3
1	1.0356-0	1.030-1	1.0319-5	9.395-4	9.427-1	9.680-1	9.563-1	9.563-1
1	1.0355-0	1.064-1	1.046-3	1.026-1	1.0313-1	9.928-1	9.775-1	9.775-1
2	1.0117-0	1.093-1	1.072-0	1.053-1	1.035-1	1.619-0	1.621-0	1.621-0
3	1.0152-0	1.126-1	1.12-0	1.081-1	1.091-1	1.647-0	1.629-0	1.629-0
4	1.0135-0	1.162-1	1.135-0	1.111-0	1.096-1	1.673-0	1.652-0	1.652-0
5	1.0133-0	1.214-0	1.214-0	1.145-1	1.121-1	1.699-0	1.673-0	1.673-0
6	1.202-0	1.214-0	4.452-0	1.164-1	1.156-1	1.131-0	1.109-0	1.109-0
7	1.230-0	1.274-0	1.233-0	1.185-1	1.223-1	1.170-0	1.142-0	1.142-0
8	1.325-0	1.255-0	1.296-0	1.245-1	1.216-1	1.211-0	1.191-0	1.191-0
9	1.975-0	1.353-0	1.238-0	1.317-0	1.259-1	1.231-0	1.210-0	1.210-0
10	1.0473-0	1.352-0	1.377-0	1.317-0	1.548-1	1.274-0	1.274-0	1.274-0
11	1.535-0	1.493-0	1.393-0	1.395-0	1.332-1	1.251-0	1.295-0	1.295-0
12	1.0614-0	1.547-0	1.57-0	1.416-1	1.425-1	1.376-0	1.270-0	1.270-0
13	1.0719-0	1.625-0	1.558-0	1.530-0	1.430-1	1.528-0	1.352-0	1.352-0
14	1.0455-0	1.729-0	1.638-0	1.571-0	1.572-1	1.444-1	1.257-0	1.257-0
15	2.172-0	1.979-0	1.741-0	1.647-0	1.546-1	1.749-0	1.659-0	1.659-0
16	2.0474-0	2.251-0	1.693-0	1.753-0	1.639-1	1.595-0	1.236-0	1.236-0
17	1.571-0	2.223-0	2.245-0	1.910-0	1.700-1	1.672-0	1.615-0	1.615-0

Table 100

2-CYANOPHENYL FINE (4(2) 2ND. +)

λ/nm	ϵ	1	2	3	4	5	6
4.194	1.0147-	1.0114-	1.0133-	1.0155-	1.0229-	1.0316-	9.501-1
4.195	1.0210-	1.0152-	1.0121-	1.0230-	1.052-J	1.036-L	9.671-1
4.233	1.0233-	1.0154-	1.0155-	1.0249-	1.099-J	1.039-Q	1.043-J
4.241	1.0249-	1.0202-	1.0143-	1.0134-	1.0137-J	1.0102-U	1.049-J
4.324	1.0324-	1.033-	1.0211-	1.0134-	1.0150-U	1.0145-U	1.0111-U
4.456	1.0456-						1.012-U

λ/nm	4	5	6	7	8	9	10
4.324	3.0329-1	8.0325-1	9.0614-1	8.0465-1	8.0392-1	9.0341-1	8.0394-1
4.641	3.0413-1	9.0413-1	9.051-1	9.023-1	8.0545-1	8.0420-1	8.0329-1
4.944	3.0716-1	9.0435-1	9.0291-1	9.0357-1	8.0847-1	8.0622-1	8.0435-1
5.222	3.0401-1	9.0733-1	9.0579-1	9.0329-1	9.0153-1	8.0345-1	8.0717-1
5.229	3.0401-1	1.033-J	9.0564-1	9.0639-1	9.0423-1	9.0216-1	9.0601-1
5.455	3.0401-1						8.0742-1

Table 10

RECENT TENTS FOR N2 3-M 17

	vV	v.	1	2	3	4	5	6	7	8	9	10
1	1.226-0	1.242-J	1.276-0	1.292-0	1.319-0	1.341-0	1.367-C	1.373-C				
2	1.216-0	1.236-0	1.270-0	1.293-0	1.314-0	1.336-0	1.361-0	1.362-0				
3	1.213-0	1.239-0	1.295-0	1.298-0	1.317-0	1.330-0	1.351-0	1.354-0				
4	1.213-0	1.225-0	1.275-0	1.292-0	1.313-0	1.332-0	1.351-0	1.354-0				
5	1.213-0	1.225-0	1.278-0	1.294-0	1.313-0	1.332-0	1.351-0	1.354-0				
6	1.213-0	1.225-0	1.278-0	1.294-0	1.313-0	1.332-0	1.351-0	1.354-0				
7	1.217-0	1.229-0	1.280-0	1.299-0	1.316-0	1.335-0	1.354-0	1.363-0				
8	1.219-0	1.231-0	1.283-0	1.293-0	1.317-0	1.336-0	1.355-0	1.364-0				
9	1.219-0	1.225-0	1.283-0	1.293-0	1.317-0	1.336-0	1.355-0	1.364-0				
10	1.219-0	1.225-0	1.283-0	1.293-0	1.317-0	1.336-0	1.355-0	1.364-0				
11	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
12	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
13	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
14	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
15	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
16	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
17	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
18	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
19	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
20	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
21	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C
22	1.196-0	1.214-0	1.249-0	1.265-0	1.281-0	1.296-0	1.312-0	1.325-0	1.339-0	1.354-0	1.369-0	1.373-C

Table I9I (cont'd)

(11121 3-4 11)

	<i>N</i>	<i>A</i>	12	13	14	15	16	17	18	19	20	21
1	1.0 3 1 5 - 0	1.0 4 1 0 - 1	1.0 4 2 2 - 0	1.0 4 3 0 - 1	1.0 4 3 5 5 - 1	1.0 4 7 2 - 1	1.0 4 9 0 - 0	1.0 5 0 7 - 0	1.0 5 2 5 - 0	1.0 5 6 2 - 0	1.0 5 6 3 - 0	1.0 5 6 2 - 0
2	1.0 3 1 5 - 1	1.0 3 1 9 - 1	1.0 4 1 5 - 0	1.0 4 3 0 - 1	1.0 4 3 5 9 - 1	1.0 4 6 9 - 1	1.0 4 8 4 - 0	1.0 5 1 0 - 0	1.0 5 1 6 - 0	1.0 5 5 5 - 0	1.0 5 3 6 - 0	1.0 5 5 5 - 0
3	1.0 3 7 0 - 1	1.0 4 2 - 0	1.0 4 1 1 - 0	1.0 4 2 7 - 0	1.0 4 4 7 - 0	1.0 4 5 9 - 1	1.0 4 7 5 - 0	1.0 4 9 9 - 0	1.0 5 2 0 - 0	1.0 5 4 9 - 0	1.0 5 1 2 - 0	1.0 5 4 9 - 0
4	1.0 3 7 5 - 1	1.0 3 9 3 - 1	1.0 4 1 4 - 0	1.0 4 1 9 - 1	1.0 4 3 4 - 0	1.0 4 5 9 - 0	1.0 4 7 1 - 0	1.0 4 9 7 - 0	1.0 5 0 3 - 0	1.0 5 3 8 - 0	1.0 5 1 9 - 0	1.0 5 1 9 - 0
5	1.0 3 7 6 - 1	1.0 3 1 2 - 1	1.0 3 9 5 - 0	1.0 4 1 9 - 1	1.0 4 3 1 - 0	1.0 4 6 7 - 0	1.0 4 6 2 - 0	1.0 4 7 6 - 0	1.0 5 0 5 - 0	1.0 5 3 2 - 0	1.0 5 1 6 - 0	1.0 5 3 2 - 0
6	1.0 3 9 6 - 1	1.0 3 7 1 - 1	1.0 3 9 3 - 0	1.0 4 1 9 - 1	1.0 4 2 3 - 0	1.0 4 3 7 - 1	1.0 4 5 1 - 0	1.0 4 7 4 - 0	1.0 4 8 9 - 0	1.0 5 1 4 - 0	1.0 5 1 4 - 0	1.0 5 1 4 - 0
7	1.0 3 9 6 - 1	1.0 3 7 1 - 1	1.0 3 9 6 - 0	1.0 4 1 9 - 1	1.0 4 3 0 - 0	1.0 4 3 5 - 0	1.0 4 5 9 - 0	1.0 4 6 5 - 0	1.0 4 6 5 - 0	1.0 5 0 2 - 0	1.0 5 1 7 - 0	1.0 5 0 2 - 0
8	1.0 3 9 6 - 1	1.0 3 6 5 - 1	1.0 3 6 5 - 0	1.0 3 7 6 - 0	1.0 3 9 9 - 0	1.0 4 1 3 - 0	1.0 4 2 7 - 0	1.0 4 4 4 - 0	1.0 4 4 4 - 0	1.0 4 9 2 - 0	1.0 5 0 2 - 0	1.0 5 0 2 - 0
9	1.0 3 9 6 - 1	1.0 3 5 5 - 1	1.0 3 7 7 - 0	1.0 3 9 1 - 0	1.0 4 5 - 0	1.0 4 2 2 - 0	1.0 4 2 2 - 0	1.0 4 3 9 - 0	1.0 4 5 4 - 0	1.0 4 9 7 - 0	1.0 5 0 4 - 0	1.0 5 0 4 - 0
10	1.0 3 9 6 - 1	1.0 3 5 5 - 1	1.0 3 7 7 - 0	1.0 3 9 1 - 0	1.0 4 5 - 0	1.0 4 1 7 - 0	1.0 4 3 1 - 0	1.0 4 4 2 - 0	1.0 4 6 7 - 0	1.0 4 8 0 - 0	1.0 4 8 0 - 0	1.0 4 8 0 - 0
11	1.0 3 9 6 - 1	1.0 3 4 9 - 1	1.0 3 0 3 - 0	1.0 3 9 3 - 0	1.0 3 9 5 - 0	1.0 4 0 9 - 0	1.0 4 4 5 - 0	1.0 4 7 3 - 0	1.0 4 9 7 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0
12	1.0 3 9 6 - 1	1.0 3 4 2 - 1	1.0 3 6 2 - 0	1.0 3 / 4 - 1	1.0 3 8 9 - 0	1.0 4 1 3 - 0	1.0 4 2 1 - 0	1.0 4 5 0 - 0	1.0 4 6 3 - 0	1.0 4 6 9 - 0	1.0 4 6 9 - 0	1.0 4 6 9 - 0
13	1.0 3 9 6 - 1	1.0 3 2 2 - 0	1.0 3 6 3 - 1	1.0 5 5 4 - 0	1.0 3 6 3 - 0	1.0 4 1 0 - 0	1.0 4 1 6 - 0	1.0 4 4 7 - 0	1.0 4 6 3 - 0	1.0 4 6 9 - 0	1.0 4 6 9 - 0	1.0 4 6 9 - 0
14	1.0 3 9 6 - 1	1.0 3 4 7 - 0	1.0 3 5 4 - 1	1.0 3 4 0 - 0	1.0 3 5 7 - 0	1.0 3 7 9 - 0	1.0 3 9 3 - 0	1.0 4 2 6 - 0	1.0 4 3 9 - 0	1.0 4 7 2 - 0	1.0 4 7 2 - 0	1.0 4 7 2 - 0
15	1.0 3 9 6 - 1	1.0 3 4 7 - 0	1.0 3 5 4 - 0	1.0 3 4 0 - 0	1.0 3 5 9 - 0	1.0 3 7 3 - 0	1.0 3 9 0 - 0	1.0 4 0 5 - 0	1.0 4 1 8 - 0	1.0 4 5 1 - 0	1.0 4 6 3 - 0	1.0 4 6 3 - 0
16	1.0 3 9 6 - 1	1.0 3 4 7 - 0	1.0 3 5 4 - 0	1.0 3 4 0 - 0	1.0 3 5 9 - 0	1.0 3 7 3 - 0	1.0 3 9 0 - 0	1.0 4 0 5 - 0	1.0 4 1 8 - 0	1.0 4 5 1 - 0	1.0 4 6 3 - 0	1.0 4 6 3 - 0
17	1.0 3 9 6 - 1	1.0 3 4 9 - 1	1.0 3 4 9 - 1	1.0 3 4 9 - 1	1.0 3 9 5 - 0	1.0 4 0 9 - 0	1.0 4 4 5 - 0	1.0 4 7 3 - 0	1.0 4 9 7 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0
18	1.0 3 9 6 - 1	1.0 3 4 9 - 1	1.0 3 4 9 - 1	1.0 3 4 9 - 1	1.0 3 9 5 - 0	1.0 4 0 9 - 0	1.0 4 4 5 - 0	1.0 4 7 3 - 0	1.0 4 9 7 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0
19	1.0 3 9 6 - 1	1.0 3 4 9 - 1	1.0 3 4 9 - 1	1.0 3 4 9 - 1	1.0 3 9 5 - 0	1.0 4 0 9 - 0	1.0 4 4 5 - 0	1.0 4 7 3 - 0	1.0 4 9 7 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0
20	1.0 3 9 6 - 1	1.0 3 4 9 - 1	1.0 3 4 9 - 1	1.0 3 4 9 - 1	1.0 3 9 5 - 0	1.0 4 0 9 - 0	1.0 4 4 5 - 0	1.0 4 7 3 - 0	1.0 4 9 7 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0
21	1.0 3 9 6 - 1	1.0 3 4 9 - 1	1.0 3 4 9 - 1	1.0 3 4 9 - 1	1.0 3 9 5 - 0	1.0 4 0 9 - 0	1.0 4 4 5 - 0	1.0 4 7 3 - 0	1.0 4 9 7 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0	1.0 4 9 9 - 0

Table I02

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Table I02 (cont'd)

(N(2) 3-4 2)

	VV	11	12	13	14	15	16	17	18	19	20	21
1.	1.0342-	1.0415-	1.0429-	1.0446-	1.0455-	1.0494-	1.0523-	1.0543-	1.0564-	1.0595-	1.0595-	1.0595-
2.	1.0416-	1.0414-	1.0422-	1.0434-	1.0434-	1.0446-	1.0496-	1.0516-	1.0536-	1.0556-	1.0556-	1.0556-
3.	1.0511-	1.0394-	1.0415-	1.0423-	1.0423-	1.0471-	1.0496-	1.0519-	1.0529-	1.0543-	1.0570-	1.0570-
4.	1.0513-	1.0391-	1.0342-	1.0429-	1.0447-	1.0455-	1.0483-	1.0512-	1.0521-	1.0541-	1.0562-	1.0562-
5.	1.0517-	1.0395-	1.0413-	1.0420-	1.0436-	1.0454-	1.0477-	1.0495-	1.0514-	1.0533-	1.0554-	1.0554-
6.	1.0559-	1.0377-	1.0399-	1.0414-	1.0431-	1.0449-	1.0465-	1.0489-	1.0509-	1.0526-	1.0546-	1.0546-
7.	1.0555-	1.0371-	1.0398-	1.0415-	1.0439-	1.0464-	1.0480-	1.0477-	1.0494-	1.0516-	1.0542-	1.0542-
8.	1.0366-	1.0353-	1.0376-	1.0403-	1.0417-	1.0433-	1.0466-	1.0473-	1.0489-	1.0516-	1.0521-	1.0521-
9.	1.0376-	1.0356-	1.0374-	1.0391-	1.0417-	1.0430-	1.0445-	1.0451-	1.0475-	1.0515-	1.0519-	1.0519-
10.	1.0333-	1.0355-	1.0367-	1.0394-	1.0412-	1.0419-	1.0433-	1.0459-	1.0473-	1.0499-	1.0498-	1.0498-
11.	1.0324-	1.0353-	1.0361-	1.0378-	1.0394-	1.0396-	1.0431-	1.0447-	1.0460-	1.0477-	1.0494-	1.0494-
12.	1.0316-	1.0329-	1.0347-	1.0364-	1.0393-	1.0393-	1.0437-	1.0454-	1.0460-	1.0474-	1.0497-	1.0497-
13.	1.0317-	1.0322-	1.0339-	1.0356-	1.0376-	1.0419-	1.0416-	1.0425-	1.0434-	1.0452-	1.0472-	1.0472-
14.	1.0312-	1.0314-	1.0334-	1.0351-	1.0379-	1.0399-	1.0462-	1.0462-	1.0473-	1.0483-	1.0493-	1.0493-
15.	1.0317-	1.0334-	1.0354-	1.0371-	1.0394-	1.0415-	1.0447-	1.0460-	1.0474-	1.0487-	1.0497-	1.0497-
16.	1.0316-	1.0329-	1.0347-	1.0364-	1.0393-	1.0419-	1.0446-	1.0466-	1.0489-	1.0516-	1.0521-	1.0521-
17.	1.0274-	1.0316-	1.0334-	1.0356-	1.0380-	1.0396-	1.0423-	1.0447-	1.0460-	1.0474-	1.0497-	1.0497-
18.	1.0275-	1.0317-	1.0335-	1.0354-	1.0381-	1.0399-	1.0424-	1.0440-	1.0455-	1.0471-	1.0493-	1.0493-
19.	1.0273-	1.0319-	1.0330-	1.0351-	1.0382-	1.0396-	1.0424-	1.0440-	1.0455-	1.0471-	1.0493-	1.0493-
20.	1.0271-	1.0314-	1.0330-	1.0359-	1.0387-	1.0397-	1.0437-	1.0454-	1.0469-	1.0485-	1.0503-	1.0503-
21.	1.0205-	1.0276-	1.0344-	1.0362-	1.0384-	1.0394-	1.0415-	1.0435-	1.0454-	1.0474-	1.0493-	1.0493-
22.	1.0201-	1.0275-	1.0314-	1.0335-	1.0356-	1.0376-	1.0406-	1.0426-	1.0445-	1.0464-	1.0483-	1.0483-
23.	1.0200-	1.0274-	1.0314-	1.0337-	1.0359-	1.0380-	1.0415-	1.0436-	1.0455-	1.0474-	1.0493-	1.0493-
24.	1.0201-	1.0276-	1.0300-	1.0334-	1.0352-	1.0374-	1.0394-	1.0413-	1.0432-	1.0451-	1.0470-	1.0470-

Table I03

R-CENTROIDS FOR (1120 MEINEL)

<i>N</i>	<i>C</i>	1	2	3	4	5	6	7	8	9	10	11	12
1	1.157-	1.1.136-	1.233-J	1.275-9	1.332-9	1.393-0	1.238-9	1.338-9	1.462-J	1.454-L	2.042-0	1.248-J	1.273-9
2	1.166-	1.1.131-	1.211-J	1.239-0	1.293-0	1.293-0	1.211-J	1.291-J	1.403-J	1.513-0	2.931-J	1.253-0	1.339-9
3	1.199-	1.1.135-	1.120-J	1.221-J	1.247-J	1.247-J	1.120-J	1.291-J	1.366-J	1.413-0	1.496-9	2.970-1	1.279-J
4	1.215-	1.1.132-	1.233-J	1.239-J	1.169-J	1.169-J	1.233-J	1.257-J	1.239-J	1.352-0	1.413-0	1.563-3	1.319-1
5	1.215-	1.1.135-	1.120-J	1.120-J	1.120-J	1.120-J	1.130-J	1.130-J	1.279-J	1.359-0	1.359-0	1.426-J	1.526-J
6	1.215-	1.1.135-	1.115-J	1.129-J	1.130-J	1.130-J	1.130-J	1.130-J	1.279-J	1.359-0	1.359-0	1.426-J	1.526-J
7	1.215-	1.1.132-	1.029-J	1.035-J	1.095-J	1.095-J	1.071-J	1.071-J	1.151-J	1.237-J	1.237-J	1.367-J	1.437-0
8	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.222-J	1.222-J	1.326-J	1.376-3
9	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
10	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
11	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
12	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
13	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
14	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
15	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
16	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
17	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
18	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
19	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3
20	1.215-	1.1.135-	1.029-J	1.035-J	1.071-J	1.071-J	1.071-J	1.071-J	1.151-J	1.230-J	1.230-J	1.320-J	1.376-3

Table I03 (cont'd)

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<i>J</i>	13	4	15	13	17	14	19	2J	21	22	23	24	25
1	1.277-4	1.029-3	1.034-3	1.019-1	1.057-2	1.042-2	1.0215-2	1.0227-2	1.0114-0	1.0236-2	1.0217-2	1.0144-1	1.0332-3
2	1.745-2	1.645-2	1.6234-3	1.6592-1	1.6256-3	1.6212-2	1.6413-2	1.6333-3	1.6578-0	1.6283-3	1.6395-3	1.6129-2	1.6241-6
3	1.0255-1	1.0149-2	1.01572-2	1.0412-1	1.0335-1	1.0756-2	1.0214-2	1.0241-3	1.0529-0	1.0225-2	1.0214-3	1.0365-1	1.0433-6
4	1.0269-1	1.0122-2	1.01223-2	1.0492-1	1.0321-2	1.0647-2	1.0295-2	1.0544-3	1.0336-0	1.0526-2	1.0467-1	1.0167-2	1.0206-0
5	1.373-6	1.213-2	1.0335-3	1.2566-4	1.2033-2	1.374-2	1.214-2	1.294-3	1.473-0	1.156-2	9.151-1	1.454-1	1.119-4
6	3.063-4	1.049-2	1.0214-2	1.0382-1	1.0279-1	1.0193-1	1.0061-1	1.0683-6	1.0154-0	1.0443-1	1.0272-3	1.0345-3	2.0367-6
7	1.0775-6	1.027-2	1.0525-2	1.0243-1	1.0243-1	1.0479-2	1.0324-2	1.0195-2	1.0617-1	1.0372-0	1.0272-1	1.0178-3	1.0314-3
8	1.0262-6	1.0135-2	1.0343-1	1.0566-3	1.0137-3	1.0280-3	1.0334-3	1.0232-0	9.359-1	1.0524-1	1.0187-4	1.0141-3	1.0151-3
9	1.0464-1	1.0274-2	1.0335-3	1.0704-1	1.0727-2	1.0450-2	1.0354-2	1.0211-2	1.0237-6	1.0152-1	1.0670-3	1.0295-3	9.303-1
10	1.0474-4	1.0167-4	1.0235-5	1.0456-3	1.0169-3	1.069-2	1.0725-3	1.0234-1	1.0249-3	1.0111-2	1.0275-3	1.0563-1	1.349-3
11	1.0415-6	1.0141-4	1.0425-3	1.0611-3	1.0772-3	1.062-2	1.0814-3	1.062-2	1.0312-1	1.0312-1	9.756-1	1.0312-3	1.281-3
12	1.0405-6	1.0149-3	1.0405-3	1.0494-3	1.0313-0	1.0168-3	1.0365-2	1.096-2	1.0372-0	1.0732-0	1.0732-1	1.0497-3	2.0277-0
13	1.0269-5	1.0171-2	1.0171-2	1.0453-4	1.0356-1	1.0637-1	1.0751-0	1.0434-1	2.0273-0	1.0496-2	1.0924-3	1.0481-3	1.324-2
14	1.0254-4	1.0171-2	1.032-2	1.0547-2	1.0451-4	1.0213-2	1.0653-3	1.0947-6	1.0523-6	1.0244-2	1.0579-3	1.0663-2	1.646-6
15	1.0265-6	1.0167-4	1.0224-3	1.0424-3	1.0111-3	1.0145-4	1.060-2	1.0530-2	1.0641-0	9.553-0	1.0568-2	1.0626-3	8.393-1
16	1.0160-6	1.0160-6	1.0449-2	1.0601-3	1.0772-3	1.062-2	1.0814-3	1.062-2	1.0312-1	1.0312-1	9.756-1	1.0312-3	1.281-3
17	1.0126-5	1.0171-2	1.0171-2	1.0453-4	1.0356-1	1.0637-1	1.0751-0	1.0434-1	2.0273-0	1.0496-2	1.0924-3	1.0481-3	1.324-2
18	1.0126-5	1.0171-2	1.032-2	1.0547-2	1.0451-4	1.0213-2	1.0653-3	1.0947-6	1.0523-6	1.0244-2	1.0579-3	1.0663-2	1.646-6
19	1.0116-5	1.0167-4	1.0224-3	1.0424-3	1.0111-3	1.0145-4	1.060-2	1.0530-2	1.0641-0	9.553-0	1.0568-2	1.0626-3	8.393-1
20	1.0116-5	1.0167-4	1.032-2	1.0547-2	1.0451-4	1.0213-2	1.0653-3	1.0947-6	1.0523-6	1.0244-2	1.0579-3	1.0663-2	1.646-6
21	1.0138-6	1.0138-6	1.0449-2	1.0601-3	1.0772-3	1.062-2	1.0814-3	1.062-2	1.0312-1	1.0312-1	9.756-1	1.0312-3	1.281-3
22	1.0138-6	1.0138-6	1.0171-2	1.0171-2	1.0453-4	1.0356-1	1.0637-1	1.0751-0	1.0434-1	2.0273-0	1.0496-2	1.0924-3	1.0481-3
23	1.0116-5	1.0116-5	1.032-2	1.0547-2	1.0451-4	1.0213-2	1.0653-3	1.0947-6	1.0523-6	1.0244-2	1.0579-3	1.0663-2	1.646-6
24	1.0116-5	1.0116-5	1.0449-2	1.0601-3	1.0772-3	1.062-2	1.0814-3	1.062-2	1.0312-1	1.0312-1	9.756-1	1.0312-3	1.281-3
25	1.0116-5	1.0116-5	1.0171-2	1.0171-2	1.0453-4	1.0356-1	1.0637-1	1.0751-0	1.0434-1	2.0273-0	1.0496-2	1.0924-3	1.0481-3

Table 104

R-CENTROIDS FOR (N2+ 1ST. NEG.)

VV	1	2	3	4	5	6	7	8	9	10
1.0105-1	1.0621-0	1.0711-0	9.0740-1	9.0439-1	9.0257-1	9.0179-1	9.017-1	8.0342-1	5.0579-1	1.0253-1
1.1.03-1	1.0111-1	1.0557-0	1.0017-1	9.0829-1	9.0517-1	9.0239-1	9.017-1	8.0309-1	6.0391-1	6.0915-1
1.2.04-1	1.0137-1	1.0304-1	1.0023-0	9.076-1	9.0564-1	9.0265-1	9.017-1	8.0979-1	6.0739-1	6.0510-1
1.2.05-1	1.0151-1	1.0304-1	1.0027-0	1.024-1	9.0912-1	9.0399-1	9.017-1	8.0317-1	6.0032-1	6.0743-1
1.3.04-1	1.0173-0	1.0275-1	1.0070-1	1.024-1	9.0912-1	9.0399-1	9.017-1	8.0317-1	6.0032-1	6.0743-1
1.4.05-1	1.0239-0	1.0161-1	9.0453-1	1.0373-1	1.034-1	9.0955-1	9.032-1	9.0351-1	9.0351-1	9.090-1
1.5.06-1	1.0461-1	1.0364-0	1.0250-1	1.035-1	1.0072-1	1.038-0	9.0992-1	9.0671-1	9.0375-1	9.0375-1
1.6.07-1	1.0214-1	1.0983-1	1.0413-1	1.0264-0	1.0211-0	9.0793-1	1.0359-0	1.0444-1	1.0011-1	9.0703-1
1.7.08-1	1.0113-1	1.0231-1	1.0019-1	1.0495-1	1.0233-1	1.0227-1	8.960-1	9.0392-1	1.0053-0	1.0053-0
1.8.09-1	1.0115-1	1.0196-1	1.0156-1	1.0475-0	1.0329-1	1.0159-1	1.0736-1	1.0245-1	5.0525-1	6.0977-1
1.9.10-1	1.0115-1	1.0115-1	1.0111-1	1.0514-0	1.0243-1	1.0286-1	1.0327-1	1.0262-1	9.0024-0	6.0234-0
1.10.11-1	1.0115-1	1.0115-1	1.0115-1	1.0396-0	1.0235-1	1.0649-1	1.0314-1	1.047-1	1.0366-1	1.0276-1
1.11.12-1	1.0115-1	1.0552-0	1.0109-1	1.0427-1	1.0322-1	1.0539-1	1.0419-1	1.0190-1	1.0465-1	1.0296-1
1.12.13-1	1.0115-1	1.0129-1	1.0071-0	1.0295-1	1.0313-1	1.0956-1	1.0464-1	1.0197-1	1.0732-1	1.0251-1
1.13.14-1	1.0115-1	1.0269-1	1.0161-0	1.0039-1	1.0117-0	1.0573-1	1.0248-1	1.0290-1	1.0373-1	1.0017-1
1.14.15-1	1.0115-1	1.0139-1	1.0163-0	1.0767-1	1.0950-1	1.0279-1	1.0076-1	1.0395-0	1.0433-0	1.0172-1
1.15.16-1	1.0115-1	1.0126-1	1.0248-1	1.0525-1	1.038-1	1.0512-1	1.0214-0	1.0942-1	1.0251-1	2.0546-0
1.16.17-1	1.0115-1	1.0117-1	1.0147-0	1.0357-1	1.0263-0	1.0265-1	1.0292-1	1.0367-1	9.0510-1	1.0372-0
1.17.18-1	1.0115-1	1.0136-1	1.0065-1	1.0310-1	1.0125-1	1.0494-1	1.0084-1	1.0206-1	1.0773-1	1.0224-0
1.18.19-1	1.0115-1	1.0149-1	1.0149-1	1.014-1	1.014-1	7.0487-1	1.0211-1	4.0025-1	8.0149-1	9.0111-1
1.19.20-1	1.0115-1	1.0271-1	1.0120-1	1.0117-0	1.0117-0	3.0199-1	1.0041-1	1.0470-1	1.0191-0	1.0225-0
1.20.21-1	1.0115-1	1.0143-1	1.0143-1	2.0569-1	1.0143-1	1.0525-1	1.0317-1	1.0284-1	7.0499-1	1.0376-1
1.21.22-1	1.0115-1	1.0143-1	1.0143-1	1.0143-1	1.0143-1	1.0317-1	1.0076-1	1.0433-0	9.0867-1	1.0433-0

Table 104 (cont'd)

1424 1511 NEG. 1

Table 105

R-CENTROIDS FOR (42+ 2ND. NEG.)

V	W	X	Y	1	2	3	4	5	6	7	8	9	10
1.0116-0	1.0213-0	1.0237-0	1.0223-0	1.0277-0	1.0304-0	1.0335-0	1.0358-0	1.0390-0	1.0342-0	1.0315-0	1.0315-0	1.0346-0	1.0258-0
1.016-0	1.0194-0	1.0211-0	1.0225-0	1.0259-0	1.0213-0	1.0213-0	1.0299-0	1.0299-0	1.0299-0	1.0347-0	1.0347-0	1.0436-0	2.0715-0
1.013-0	1.0174-0	1.0139-0	1.0213-0	1.0239-0	1.0229-0	1.0229-0	1.0199-0	1.0199-0	1.0199-0	1.0347-0	1.0347-0	1.0437-0	1.0437-0
1.018-0	1.019-0	1.0199-0	1.0195-0	1.0195-0	1.0195-0	1.0195-0	1.0239-0	1.0239-0	1.0239-0	1.0325-0	1.0325-0	1.0353-0	1.0402-0
1.01-0	1.01-0	1.01-0	1.0176-0	1.0176-0	1.0211-0	1.0211-0	1.0266-0	1.0266-0	1.0252-0	1.0220-0	1.0220-0	1.0342-0	1.0361-0
1.0135-0	1.015-0	1.015-0	1.0158-0	1.0158-0	1.0181-0	1.0181-0	1.0172-0	1.0172-0	1.0172-0	1.0212-0	1.0212-0	1.0249-0	1.0249-0
1.015-0	1.015-0	1.015-0	1.0136-0	1.0136-0	1.0163-0	1.0163-0	1.0147-0	1.0147-0	1.0193-0	1.0224-0	1.0224-0	1.0275-0	1.0275-0
1.01-0	1.01-0	1.01-0	1.0120-0	1.0120-0	1.0140-0	1.0140-0	1.0135-0	1.0135-0	1.0129-0	1.0196-0	1.0196-0	1.0230-0	1.0230-0
1.01-0	1.01-0	1.01-0	1.0051-0	1.0051-0	1.0149-0	1.0149-0	1.0151-0	1.0151-0	1.0173-0	1.0176-0	1.0203-0	1.0236-0	1.0236-0
1.01-0	1.01-0	1.01-0	1.0112-0	1.0112-0	1.0113-0	1.0113-0	1.0129-0	1.0129-0	1.0131-0	1.0213-0	1.0182-0	1.0212-0	1.0212-0
1.01-0	1.01-0	1.01-0	1.0092-0	1.0092-0	1.0118-0	1.0118-0	1.0144-0	1.0144-0	1.0160-0	1.0160-0	1.0160-0	1.0146-0	1.0146-0
1.	1.	1.	1.	1.	1.	1.	1.	1.	1.	1.	1.	1.	1.

V	W	X	Y	11	12	13	14	15	16	17	18	19	20
1.0313-0	1.0443-0	1.0569-0	1.0449-0	1.0672-0	1.0236-0	2.0227-0	1.0351-0	2.0191-1	1.0562-0	1.0191-1	1.0480-0	1.0155-0	1.0155-0
1.033-0	1.0737-0	1.0224-0	1.0734-0	1.0248-0	2.0217-0	1.0322-0	3.0621-1	1.0346-0	1.0346-0	1.0346-0	1.0724-0	1.0724-0	1.0724-0
2.0452-0	1.0335-0	1.0981-0	1.0299-0	2.0219-0	1.0324-0	1.0259-0	1.0426-0	1.0426-0	1.0426-0	1.0426-0	1.0550-0	1.0550-0	1.0550-0
3.051-0	1.0433-0	1.0305-0	2.0847-0	1.0341-0	1.0362-0	1.0304-0	6.0623-1	1.0472-0	1.0472-0	1.0472-0	1.0620-0	1.0620-0	1.0620-0
4.0462-0	1.0522-0	1.0165-1	1.0394-0	1.0347-0	1.0394-0	0.0110-1	1.0442-0	9.0934-1	1.0592-0	1.0592-0	1.045-0	1.045-0	1.045-0
5.0375-0	1.0416-0	1.0536-0	2.0390-1	1.0423-0	2.0399-1	1.0442-0	1.0442-0	1.0442-0	1.0442-0	1.0442-0	1.0513-0	1.0513-0	1.0513-0
6.0421-0	1.0337-0	1.0423-0	1.0551-0	9.0524-1	1.0454-0	9.0154-1	1.0454-0	1.0454-0	1.0454-0	1.0454-0	1.0443-0	1.0443-0	1.0443-0
7.0429-0	1.0312-0	1.0395-0	1.0431-0	1.0553-0	1.0553-0	3.0729-1	1.0457-0	1.0457-0	1.0457-0	1.0457-0	1.0591-0	1.0591-0	1.0591-0
8.0427-0	1.0259-0	1.0259-0	7.0621-1	1.0409-0	1.0409-0	1.0531-0	1.0531-0	1.0531-0	1.0531-0	1.0531-0	1.0485-0	1.0485-0	1.0485-0
9.0423-0	1.0229-0	1.0229-0	1.0275-0	1.0372-0	1.0372-0	1.0422-0	1.0422-0	1.0422-0	1.0422-0	1.0422-0	1.0562-0	1.0562-0	1.0562-0
10.0421-0	1.0213-0	1.0213-0	1.0250-0	1.0236-0	1.0236-0	1.0246-0	1.0246-0	1.0246-0	1.0246-0	1.0246-0	1.0129-0	1.0129-0	1.0129-0
11.	1.	1.	1.	1.	1.	1.	1.	1.	1.	1.	1.	1.	1.

Table I06

112 : विक्रम का स्वीकृति-

Table 106 (cont'd)
 (10 GAMA(1/2))

	11	10	9	11	12	13	14	15	16	17
v	3.163-1	3.163-1	3.163-1	3.093-1	3.752-1	3.635-1	3.555-1	3.559-1	3.161-1	
1	3.540-1	3.318-1	3.236-1	3.093-1	3.953-1	3.824-1	3.935-1	3.253-1	3.353-1	
2	3.777-1	3.615-1	3.405-1	3.311-1	3.123-1	3.119-1	3.087-1	3.777-1	3.531-1	
3	3.622-1	3.547-1	3.634-1	3.529-1	3.379-1	3.234-1	3.031-1	3.455-1	3.796-1	
4	3.624-1	3.579-1	3.514-1	3.724-1	3.537-1	3.447-1	3.301-1	3.159-1	3.019-1	
5	3.2-5-2	3.37-6	3.017-1	3.910-1	3.825-1	3.638-1	3.516-1	3.379-1	3.228-1	
6	3.174-5	3.48-5	3.558-3	3.025-1	3.016-1	3.896-1	3.739-1	3.584-1	3.442-1	
7	3.184-6	3.392-5	3.565-3	3.031-5	3.039-5	3.014-6	3.959-1	3.810-1	3.660-1	
8	3.120-5	3.131-0	3.032-3	3.69-5	3.049-3	3.914-1	3.924-0	3.035-1	3.894-1	
9	3.162-5	3.132-3	3.066-3	3.114-6	3.078-3	3.028-3	3.038-0	3.047-3	3.013-5	
10	3.142-5	3.143-6	3.144-3	3.139-0	3.135-0	3.089-0	3.067-0	3.049-9	3.030-0	
11	3.234-5	3.196-5	3.222-3	3.155-6	3.124-0	3.026-3	3.115-0	3.078-9	3.058-0	
12	3.202-5	3.249-5	3.249-3	3.149-3	3.168-3	3.135-0	3.103-0	3.151-0	3.091-3	
13	3.315-5	3.271-5	3.331-3	3.220-5	3.131-5	3.189-3	3.148-0	3.119-3	3.059-3	
14	3.341-5	3.31-6	3.31-3	3.243-6	3.234-0	3.197-0	3.573-0	3.161-3	3.132-9	
15	3.391-5	3.351-0	3.3-9-3	3.234-6	3.263-0	3.248-3	3.212-0	3.169-3	3.143-0	
16	3.422-5	3.392-0	3.371-3	3.334-3	3.278-3	3.274-3	3.255-0	3.226-1	3.199-3	

Table 107

R-CENTROIDS FOR NCA (3/?)

ν	$\nu\nu$	ν	1	2	3	4	5	6	7	8
-	1.113-3	1.0933-1	1.075-1	1.054-1	1.041-1	1.026-1	1.012-1	9.997-1	9.859-1	
1	1.154-3	1.115-3	1.067-1	1.035-1	1.015-1	1.006-1	1.032-1	1.018-1	1.014-1	
2	1.154-3	9.455-1	1.123-1	1.111-1	1.079-1	1.067-1	1.056-1	1.039-1	1.024-1	
3	1.152-1	1.173-3	1.144-1	1.134-1	1.113-1	1.086-1	1.057-1	1.042-1	1.034-1	
4	1.225-1	1.216-1	1.217-1	1.193-1	1.124-1	1.126-1	1.096-1	1.076-1	1.056-1	
5	1.266-1	1.231-1	1.239-1	1.171-1	1.154-1	1.135-1	1.115-1	1.109-1	1.094-1	
6	1.345-1	1.256-1	1.234-1	1.221-1	1.143-1	1.216-1	1.144-1	1.115-1	9.795-1	
7	1.345-1	1.346-1	1.273-1	1.246-1	1.447-1	1.193-1	1.252-1	1.156-1	1.127-1	
8	1.346-1	1.349-1	1.322-1	1.279-1	1.254-1	1.210-1	1.203-1	1.168-1	1.212-1	
9	1.423-1	1.394-1	1.355-1	1.313-1	1.236-1	1.264-1	1.224-1	1.219-1	1.179-1	
10	1.544-1	1.431-1	1.396-1	1.359-1	1.323-1	1.293-1	1.297-1	1.234-1	1.213-1	
11	1.547-1	1.450-1	1.426-1	1.399-1	1.354-1	1.329-1	1.300-1	1.247-1	1.244-1	
12	1.274-1	1.425-1	1.444-1	1.429-1	1.413-1	1.369-1	1.336-1	1.308-1	1.253-1	
13	1.313-1	1.411-1	1.411-1	1.457-1	1.436-1	1.436-1	1.375-1	1.343-1	1.317-1	
14	1.221-1	1.164-1	1.75-1	1.515-1	1.470-1	1.443-1	1.414-1	1.381-1	1.350-1	
15	1.429-1	1.251-1	1.179-1	1.029-1	1.535-1	1.460-1	1.450-1	1.423-1	1.339-1	
16	1.205-1	1.197-1	1.21-1	1.793-1	1.652-1	1.535-1	1.496-1	1.457-1	1.429-1	

Table 107 (cont'd)

(NO GA14A(3/2))

VV	9	10	11	12	13	14	15	16	17
1	9.736-1	9.019-1	9.578-1	9.473-1	9.313-1	9.207-1	9.114-1	9.019-1	9.913-1
2	9.915-2	9.793-1	9.5975-1	9.565-1	9.459-1	9.356-1	9.257-1	9.161-1	9.064-1
3	1.0641-1	9.972-1	9.349-1	9.733-1	9.622-1	9.514-1	9.416-1	9.309-1	9.210-1
4	1.0651-1	1.016-0	1.03-3-1	9.977-1	9.719-1	9.577-1	9.270-1	9.466-1	9.364-1
5	7.791-1	1.341-1	1.023-1	1.019-0	9.906-1	9.445-1	9.732-1	9.024-1	9.521-1
6	1.0656-2	1.037-0	9.341-1	1.033-0	1.016-0	1.003-0	9.906-1	9.790-1	9.691-1
7	1.0646-2	1.0374-0	1.056-0	1.034-0	9.360-1	1.026-0	1.010-0	9.967-1	9.853-1
8	1.0110-2	1.0127-0	1.053-0	1.054-0	1.049-0	1.031-0	9.059-1	1.019-0	1.073-0
9	1.0136-2	1.0111-0	1.0579-0	1.050-0	1.073-0	1.056-0	1.041-0	1.025-0	7.625-1
10	1.0135-2	1.0150-0	1.0121-0	1.097-0	1.026-0	1.086-0	1.065-0	1.049-1	1.035-0
11	1.0139-2	1.0137-0	1.0219-0	1.032-0	1.016-0	1.003-0	1.0177-0	1.076-0	1.058-0
12	1.0121-0	1.0204-0	1.0169-0	1.025-0	1.046-0	1.016-0	1.036-0	1.066-0	1.043-0
13	1.0254-2	1.0217-0	1.0232-0	1.031-0	1.049-0	1.024-0	1.031-0	1.007-0	1.045-0
14	1.0215-2	1.0258-0	1.0230-0	1.039-0	1.0193-0	1.062-0	1.0121-0	1.051-0	1.119-0
15	1.0343-3	1.0238-0	1.0330-0	1.0242-0	1.0210-0	1.0215-0	1.0173-0	1.043-0	1.133-0
16	1.0354-1	1.0299-0	1.0293-0	1.0269-0	1.0255-0	1.0220-0	1.0393-0	1.0198-1	1.156-0
17	1.0398-2	1.0374-1	1.0298-1	1.0271-0	1.0293-1	1.0266-0	1.0235-0	1.0190-1	1.210-1

Table 108

2-CENTROIDS FOR (NU BETA)

V	VV	4	1	2	3	4	5	6	7	8
0	1.270-1	1.296-0	1.3-3-J	1.320-0	1.337-J	1.355-0	1.373-0	1.393-0	1.412-0	
1	1.261-0	1.277-0	1.293-0	1.319-0	1.326-0	1.344-0	1.361-0	1.379-0	1.395-0	
2	1.252-1	1.264-0	1.244-0	1.261-0	1.316-0	1.333-0	1.348-0	1.358-0	1.375-0	
3	1.244-1	1.259-0	1.244-J	1.239-0	1.316-0	1.320-0	1.349-0	1.360-0	1.376-0	
4	1.236-1	1.251-0	1.251-L	1.251-L	1.295-0	1.326-0	1.332-0	1.347-0	1.353-0	
5	1.228-0	1.242-0	1.257-0	1.272-0	1.273-J	1.317-0	1.321-0	1.333-0	1.363-0	
6	1.225-1	1.234-0	1.249-J	1.262-0	1.293-0	1.296-0	1.319-0	1.335-0	1.346-0	
7	1.213-1	1.227-0	1.241-J	1.243-0	1.273-0	1.286-0	1.412-0	1.321-0	1.334-0	
8	1.205-0	1.219-0	1.232-0	1.253-0	1.264-0	1.275-0	1.298-0	1.310-0	1.313-0	
9	1.193-1	1.212-0	1.223-0	1.243-0	1.255-0	1.320-0	1.247-0	1.299-0	1.322-0	
10	1.192-1	1.205-0	1.195-0	1.235-0	1.246-0	1.257-0	1.277-0	1.454-0	1.310-0	
11	1.195-0	1.198-0	1.219-0	1.227-0	1.233-0	1.257-0	1.257-0	1.289-0	1.300-0	
12	1.179-0	1.191-0	1.211-0	1.220-0	1.247-0	1.246-0	1.268-0	1.279-0	1.296-0	
13	1.172-0	1.175-0	1.201-0	1.212-0	1.231-0	1.240-0	1.255-0	1.270-0	1.354-0	
14	1.160-0	1.170-0	1.194-0	1.215-0	1.223-0	1.232-0	1.252-0	1.260-0	1.292-0	
15	1.155-0	1.174-0	1.186-0	1.193-0	1.216-0	1.219-0	1.243-0	1.247-0	1.272-0	
16	1.154-0	1.165-0	1.182-0	1.182-0	1.219-0	1.238-0	1.235-0	1.271-0	1.263-0	
17	1.144-0	1.160-0	1.176-0	1.191-0	1.223-0	1.226-0	1.226-0	1.248-0	1.254-0	
18	1.143-0	1.154-0	1.173-0	1.184-0	1.176-0	1.212-0	1.220-0	1.239-0	1.243-0	

TABLE I
108 (cont'd)

v_v	9	10	11	12	13	14	15	16
1	1.0 41 2-3	1.0 43 3-3	1.0 45 4-3	1.0 47 5-3	1.0 50 6-3	1.0 52 5-3	1.0 55 0-3	1.0 57 7-3
1	1.0 33 5-3	1.0 43 3-3	1.0 44 4-3	1.0 46 4-3	1.0 48 5-3	1.0 50 9-3	1.0 53 4-3	1.0 56 4-3
2	1.0 39 0-3	1.0 44 1-3	1.0 42 6-3	1.0 44 3-3	1.0 46 6-3	1.0 49 6-3	1.0 51 9-3	1.0 54 3-3
3	1.0 37 6-3	1.0 33 7-3	1.0 42 5-3	1.0 43 7-3	1.0 45 5-3	1.0 47 2-3	1.0 52 5-3	1.0 53 3-3
4	1.0 35 3-3	1.0 33 9-3	1.0 43 4-3	1.0 41 9-3	1.0 48 4-3	1.0 46 7-3	1.0 43 5-3	1.0 50 2-3
5	1.0 35 3-3	1.0 37 3-3	1.0 36 7-3	1.0 38 7-3	1.0 41 9-3	1.0 43 1-3	1.0 44 7-3	1.0 49 3-3
6	1.0 34 6-3	1.0 35 3-3	1.0 36 7-3	1.0 37 1-3	1.0 38 3-3	1.0 41 5-3	1.0 42 6-3	1.0 47 3-3
7	1.0 33 4-3	1.0 36 7-3	1.0 36 7-3	1.0 37 1-3	1.0 39 1-3	1.0 41 5-3	1.0 42 6-3	1.0 47 4-3
8	1.0 32 3-3	1.0 34 5-3	1.0 34 5-3	1.0 35 7-3	1.0 39 1-3	1.0 39 6-3	1.0 40 5-3	1.0 43 9-3
9	1.0 32 2-3	1.0 33 3-3	1.0 33 3-3	1.0 23 5-3	1.0 16 3-3	1.0 38 1-3	1.0 41 1-3	1.0 45 1-3
10	1.0 31 0-3	1.0 32 5-3	1.0 32 5-3	1.0 34 5-3	1.0 35 6-3	1.0 39 5-3	1.0 39 3-3	1.0 40 6-3
11	1.0 31 0-3	1.0 33 4-3	1.0 33 4-3	1.0 33 5-3	1.0 33 5-3	1.0 36 8-3	1.0 37 7-3	1.0 40 7-3
12	1.0 29 9-3	1.0 31 1-3	1.0 32 1-3	1.0 32 1-3	1.0 34 7-3	1.0 35 5-3	1.0 41 5-3	1.0 39 0-3
13	1.0 35 4-3	1.0 36 5-3	1.0 36 5-3	1.0 36 1-3	1.0 33 3-3	1.0 33 9-3	1.0 36 7-3	1.0 37 5-3
14	1.0 29 2-3	1.0 29 2-3	1.0 29 2-3	1.0 31 4-3	1.0 32 2-3	1.0 35 5-3	1.0 35 4-3	1.0 40 4-3
15	1.0 27 2-3	1.0 27 5-3	1.0 30 1-3	1.0 30 1-3	1.0 33 3-3	1.0 33 3-3	1.0 34 1-3	1.0 37 3-3
16	1.0 26 3-3	1.0 31 6-3	1.0 29 1-3	1.0 37 3-3	1.0 32 2-3	9.0 29 1-1	1.0 35 3-3	1.0 31 3-3
17	1.0 25 4-3	1.0 27 0-3	1.0 24 2-3	1.0 30 4-3	1.0 31 1-3	1.0 33 4-3	1.0 34 1-3	1.0 36 7-3
18	1.0 24 3-3	1.0 29 0-3	1.0 26 9-3	1.0 29 3-3	1.0 29 6-3	1.0 32 2-3	1.0 31 6-3	1.0 35 3-3

Table 109

2-CENTROIDS FOR (NO DELTA (1/2))

	VV	U	W	X	Y	Z	2	3	4	5	6	7	8	9	10	11
1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1	1.0112-1
2	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1	1.0137-1
3	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1	1.0157-1
4	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1	1.0177-1
5	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1	1.0211-1
6	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1	1.0241-1

	VV	U	W	X	Y	Z	14	15	16	17	18	19	20	21	22	23
1	9.0644-1	9.0583-1	9.0315-1	9.0124-1	9.0133-1	9.0343-1	9.0359-1	9.0756-1	9.0779-1	9.0922-1	9.0944-0	1.0111-0				
2	9.1416-1	9.0935-1	9.0314-1	9.0244-1	9.0246-1	9.0192-1	9.0197-1	9.0559-1	9.0562-1	9.0564-1	9.0565-1	9.0599-1				
3	9.4205-1	9.2811-1	9.0361-1	9.0511-1	9.0511-1	9.0455-1	9.0455-1	9.0539-1	9.0539-1	9.0539-1	9.0539-1	9.0539-1	9.0539-1	9.0539-1	9.0539-1	9.0539-1
4	9.6344-1	9.0511-1	9.0341-1	9.0422-1	9.0422-1	9.0907-1	9.0532-1	9.0532-1	9.0532-1	9.0532-1	9.0532-1	9.0655-0	9.0655-0	9.0655-0	9.0655-0	9.0655-0
5	9.8133-1	9.0744-1	9.0404-1	9.0540-1	9.0540-1	9.0211-1	9.0491-1	9.0714-1	9.0714-1	9.0714-1	9.0714-1	9.0439-1	9.0439-1	9.0439-1	9.0439-1	9.0439-1

Table II0

2-CENTRAL FCG (NC DELTA (3/2))

VV	2	1	2	3	4	5	6	7	8	9	10	11
Y	1.1 3-1	1.0 81-1	1.0 863-1	1.0 135-1	1.0 337-1	1.0 333-1	1.0 47-1	1.0 23-1	1.0 624-1	9.0 469-1	9.0 291-1	9.0 137-1
+	1.1 1,7-	1.1 11-	1.1 15-	1.1 21-	1.1 37-	1.1 37-	1.0 39-	1.0 39-	1.0 617-1	9.0 975-1	9.0 748-1	9.0 591-1
2	1.1 1,7-	1.1 15-	1.1 21-	1.1 35-	1.1 39-	1.1 39-	1.0 56-	1.0 56-	1.0 628-1	1.0 012-1	1.0 367-1	1.0 652-1
3	1.2 2,1-	1.1 17-	1.1 32-	1.1 35-	1.1 33-	1.1 35-	1.0 32-	1.0 32-	1.0 142-0	1.0 634-0	1.0 118-0	1.0 022-0
4	1.2 4,6-	1.2 1-	1.1 92-	1.1 49-	1.1 21-	1.1 14-	1.0 114-	1.0 114-	1.0 656-1	1.0 666-1	1.0 442-0	1.0 323-0
VV	12	13	14	15	16	17	18	19	20	21	22	23
Y	9.6 3-1	3.9 35-1	8.0 806-1	8.0 464-1	7.0 573-1	2.0 572-1	1.0 144-0	1.0 655-0	1.0 079-0	9.0 579-1	9.0 162-1	4.0 557-1
1	9.2 18-1	9.0 22-	9.0 928-1	9.0 612-1	9.0 302-1	7.0 545-1	3.0 510-1	1.0 221-0	1.0 062-0	1.0 116-0	9.0 904-1	9.0 684-1
2	9.4 16-1	9.0 36-	9.0 137-1	9.0 540-1	9.0 173-1	7.0 269-1	3.0 876-1	1.0 244-0	1.0 019-0	1.0 273-0	9.0 923-1	1.0 019-0
3	9.7 20-1	9.0 25-	9.0 391-1	9.0 199-1	9.0 929-1	9.0 191-1	7.0 192-1	1.0 995-1	1.0 436-1	1.0 102-0	1.0 124-0	1.0 124-0
4	9.9 27-1	9.0 77-	9.0 617-1	9.0 440-1	9.0 257-1	9.0 335-1	3.0 751-1	9.0 335-1	7.0 537-1	4.0 693-1	1.0 976-0	1.0 162-0

Table III

2-CENT 2010 F72 (NO EPS) NCT (1/2)

V	VV	2	3	4	5	6	7	8	9	10	11
1	1.179-1	1.0.587-3	1.0.696-0	1.0.J+4-3	1.0.333J-3	1.0.115-1	2.0.399-1	3.0.852-1	9.0.731-1	9.0.512-1	9.0.327-1
2	1.160-1	1.0.514-3	1.0.129-3	1.0.172-3	1.0.355-3	1.0.437-3	1.0.122-3	1.0.075-3	1.0.919-1	9.0.773-1	9.0.542-1
3	1.160-1	1.0.152-3	1.0.119-3	1.0.192-3	1.0.123-3	1.0.155-3	1.0.643-3	1.0.526-3	1.0.011-3	9.0.761-1	9.0.526-1
4	1.194-1	1.0.247-3	1.0.149-3	1.0.431-3	1.0.112-3	1.0.476-3	1.0.J12-0	1.0.034-4	1.0.033-0	1.0.117-6	1.0.032-6
5	1.254-1	1.0.265-3	1.0.192-3	1.0.152-3	1.0.659-3	1.0.113-3	1.0.036-0	1.0.032-3	8.0.797-1	1.0.344-3	1.0.024-3
6	1.254-1	1.0.231-3	1.0.211-3	1.0.157-3	1.0.152-3	1.0.129-3	1.0.459-0	1.0.427-3	1.0.072-0	1.0.149-3	1.0.133-3
7	1.32-1	1.0.274-3	1.0.244-3	1.0.219-3	1.0.193-3	1.0.215-3	1.0.1472-3	1.0.144-0	1.0.065-3	1.0.115-0	1.0.034-0
8	1.32-1	1.0.311-3	1.0.3-4-3	1.0.278-3	1.0.251-3	1.0.251-3	1.0.142-0	1.0.158-3	1.0.126-0	1.0.192-0	1.0.173-0

V	VV	12	13	14	15	16	17	18	19	20	21	22	23
1	9.0.172-1	9.0.435-1	9.0.354-1	9.0.323-1	9.0.859-1	9.0.344-1	9.0.344-1	9.0.730-1	9.0.643-1	9.0.195-1	9.0.359-1	9.0.327-0	
2	9.0.315-1	9.0.275-1	9.0.157-1	9.0.132-1	9.0.848-1	9.0.399-1	9.0.411-1	7.0.953-1	6.0.145-1	2.0.353-0	1.0.143-0	1.0.28-0	
3	9.0.574-1	9.0.52-1	9.0.328-1	9.0.139-1	9.0.354-1	9.0.497-1	9.0.471-1	3.0.532-1	7.0.928-1	6.0.577-1	9.0.263-1	1.0.153-0	
4	9.0.72-1	9.0.52-1	9.0.437-1	9.0.371-1	9.0.243-1	9.0.465-1	9.0.348-1	3.0.754-1	8.0.479-1	7.0.995-1	6.0.566-1	3.0.103-0	
5	9.0.936-1	9.0.505-1	9.0.575-1	9.0.555-1	9.0.424-1	9.0.295-1	9.0.139-1	3.0.015-1	8.0.959-1	8.0.514-1	7.0.945-1	0.0.125-1	
6	9.0.112-1	9.0.101-1	9.0.361-1	9.0.732-1	9.0.609-1	9.0.494-1	9.0.352-1	9.0.277-1	9.0.043-1	6.0.342-1	6.0.553-1	d.0.209-1	
7	9.0.801-1	9.0.74-1	9.0.319-3	9.0.335-1	9.0.735-1	9.0.604-1	9.0.200-1	9.0.417-1	9.0.271-1	9.0.133-1	8.0.819-1	9.0.591-1	
8	9.0.601-1	9.0.25-1	1.0.033-3	1.0.152-3	1.0.631-3	1.0.473-3	1.0.734-1	1.0.506-1	9.0.466-1	9.0.334-1	9.0.193-1	8.0.389-1	

Table II/2

R-CENTROIDS FOR NO EPSILON (7/21)

VV	1	2	3	4	5	6	7	8	9	10	11
1	1.013-0	1.0284-1	1.0169-3	1.0356-3	1.0033-0	1.0217-3	1.0123-0	1.0091-1	9.0741-1	9.0510-1	9.0365-1
2	1.0135-0	1.0215-1	1.0453-1	1.0457-1	1.0556-1	1.0539-1	1.0523-0	1.0514-0	9.0935-1	9.0410-1	9.0543-1
3	1.0152-1	1.0215-1	1.0119-1	1.0133-1	1.0052-0	1.0071-1	1.0045-0	1.0028-0	9.0937-1	9.0533-1	9.0723-1
4	1.0193-1	1.0217-1	1.0146-0	1.0136-1	1.0113-1	1.0179-1	1.0139-0	1.0157-0	1.0035-0	1.0119-1	1.0305-1
5	1.0263-1	1.0205-1	1.0143-0	1.0152-1	1.0096-0	1.0114-0	1.0097-0	1.0084-0	1.0119-0	1.0154-1	1.0126-0
6	1.0259-1	1.0239-1	1.0210-1	1.0173-1	1.0162-1	1.0131-1	1.0122-0	1.0050-0	1.0074-0	1.0152-1	1.0119-1
7	1.0326-0	1.0277-0	1.0274-1	1.0243-0	1.0214-1	1.0192-0	1.0173-1	1.0145-0	1.0119-0	1.0196-0	1.0063-0
8	1.0326-0	1.0305-1	1.0277-0	1.0243-1	1.0212-1	1.0205-1	1.0196-1	1.0157-0	1.0126-0	1.0133-0	1.0075-0

VV	12	13	14	15	16	17	18	19	20	21	22	23
1	9.0204-1	9.0171-1	9.0069-1	9.0324-1	9.0643-1	9.0222-1	7.0391-1	1.0021-0	1.0551-0	1.0132-0	1.0006-0	9.0361-1
2	9.0443-1	9.0291-1	9.0173-1	9.0043-1	9.0913-1	9.0745-1	9.0494-1	9.0504-1	6.0444-1	2.0557-0	1.0140-0	1.0034-0
3	9.0535-1	9.0471-1	9.0345-1	9.0219-1	9.0089-1	9.0344-1	9.0765-1	9.0519-1	6.0036-1	3.0590-1	3.0465-0	1.0142-0
4	9.0751-1	9.0543-1	9.0524-1	9.0394-1	9.0266-1	9.0152-1	9.0977-1	9.0767-1	6.0520-1	5.0342-1	6.0667-1	4.0331-0
5	9.0911-1	9.0521-1	9.0703-1	9.0578-1	9.0452-1	9.0313-1	9.0178-1	9.0022-1	6.0832-1	6.0562-1	6.0074-1	6.0625-1
6	1.0019-1	1.0019-1	1.0017-1	9.0757-1	9.0633-1	9.0210-1	9.0379-1	9.0235-1	9.0074-1	6.0971-1	6.0636-1	6.0115-1
7	1.0005-1	1.0021-1	1.0013-1	9.0323-1	9.0422-1	9.0039-1	9.0565-1	9.0441-1	9.0375-1	9.0142-1	6.0934-1	6.0641-1
8	1.0003-1	1.0035-1	1.0034-1	1.0115-1	1.0033-1	9.0361-1	9.0754-1	9.0623-1	9.0496-1	9.0215-1	9.0241-1	9.0241-1

Table III3

NOT-CENTERED FOR (NO DELTA PRIMES (1/2))

VV	1	2	3	4	5	6	7	8	9	10	11
1	1.0242-1	1.0242-1	1.0271-1	1.0292-1	1.0321-1	1.0349-1	1.0376-1	1.0416-1	1.0433-0	1.0464-0	1.0499-0
2	1.0247-1	1.0243-1	1.0254-0	1.0270-1	1.0311-1	1.0332-1	1.0352-0	1.0385-1	1.0413-0	1.0443-0	1.0473-0
3	1.0242-1	1.0242-1	1.0230-1	1.0256-1	1.0296-1	1.0311-1	1.0342-0	1.0376-0	1.0395-1	1.0423-1	1.0452-0
4	1.0242-1	1.0242-1	1.0228-1	1.0242-1	1.0292-1	1.0311-1	1.0342-1	1.0376-0	1.0395-1	1.0423-1	1.0452-0
5	1.0247-1	1.0247-1	1.0229-0	1.0243-1	1.0299-1	1.0321-1	1.0352-0	1.0385-1	1.0416-0	1.0446-1	1.0476-0
6	1.0242-1	1.0242-1	1.0235-1	1.0251-1	1.0285-1	1.0312-1	1.0351-0	1.0387-1	1.0394-0	1.0433-0	1.0444-0
7	1.0247-1	1.0247-1	1.0241-1	1.0247-1	1.0292-1	1.0321-1	1.0351-0	1.0387-1	1.0394-0	1.0433-0	1.0444-0
8	1.0242-1	1.0242-1	1.0247-1	1.0253-1	1.0298-1	1.0311-1	1.0354-0	1.0391-1	1.0394-0	1.0433-0	1.0444-0
9	1.0247-1	1.0247-1	1.0251-1	1.0257-1	1.0292-1	1.0321-1	1.0351-0	1.0387-1	1.0394-0	1.0433-0	1.0444-0
10	1.0242-1	1.0242-1	1.0247-1	1.0253-1	1.0298-1	1.0311-1	1.0354-0	1.0391-1	1.0394-0	1.0433-0	1.0444-0
11	1.0247-1	1.0247-1	1.0251-1	1.0257-1	1.0292-1	1.0321-1	1.0351-0	1.0387-1	1.0394-0	1.0433-0	1.0444-0

VV	12	13	14	15	16	17	18	19	20	21	22	23
1	1.0222-1	1.0233-1	2.0249-0	1.0334-1	1.0349-1	1.0365-0	1.0382-0	1.0409-0	1.0436-0	1.0466-0	1.0493-0	1.0523-0
2	1.0222-1	1.0237-1	1.0257-1	1.0267-1	1.0317-1	1.0329-1	1.0346-0	1.0367-0	1.0389-0	1.0411-0	1.0434-0	1.0459-0
3	1.0222-1	1.0239-1	1.0255-1	1.0261-1	1.0309-1	1.0319-1	1.0337-0	1.0355-0	1.0374-0	1.0397-0	1.0415-0	1.0447-0
4	1.0222-1	1.0241-1	1.0252-1	1.0258-1	1.0304-1	1.0314-1	1.0331-0	1.0349-0	1.0367-0	1.0385-0	1.0403-0	1.0424-0
5	1.0222-1	1.0242-1	1.0252-1	1.0258-1	1.0304-1	1.0314-1	1.0331-0	1.0349-0	1.0367-0	1.0385-0	1.0403-0	1.0424-0
6	1.0222-1	1.0243-1	1.0253-1	1.0259-1	1.0305-1	1.0315-1	1.0332-0	1.0350-0	1.0368-0	1.0386-0	1.0404-0	1.0425-0
7	1.0222-1	1.0244-1	1.0254-1	1.0260-1	1.0306-1	1.0316-1	1.0333-0	1.0351-0	1.0369-0	1.0387-0	1.0405-0	1.0426-0
8	1.0222-1	1.0245-1	1.0255-1	1.0261-1	1.0307-1	1.0317-1	1.0334-0	1.0352-0	1.0370-0	1.0388-0	1.0406-0	1.0427-0
9	1.0222-1	1.0246-1	1.0256-1	1.0262-1	1.0308-1	1.0318-1	1.0335-0	1.0353-0	1.0371-0	1.0389-0	1.0407-0	1.0428-0
10	1.0222-1	1.0247-1	1.0257-1	1.0263-1	1.0309-1	1.0319-1	1.0336-0	1.0354-0	1.0372-0	1.0390-0	1.0408-0	1.0429-0
11	1.0222-1	1.0248-1	1.0258-1	1.0264-1	1.0310-1	1.0320-1	1.0337-0	1.0355-0	1.0373-0	1.0391-0	1.0409-0	1.0430-0

NOT REPRODUCIBLE

Table II4

R-CENTROIDS FOR NC 3ETA 3RIE (3/2)

VW	1	2	3	4	5	6	7	8	9	10	11	
V	1.213-1	1.246-1	1.272-0	1.297-0	1.323-0	1.349-1	1.377-0	1.405-0	1.436-0	1.465-0	1.531-0	
1	1.127-1	1.232-1	1.255-0	1.277-0	1.311-0	1.333-1	1.359-0	1.387-0	1.415-0	1.444-0	1.507-0	
2	1.0112-	1.0213-	1.0236-0	1.0257-0	1.0249-0	1.0312-1	1.0357-0	1.0371-0	1.0366-0	1.0424-0	1.0454-0	
3	1.173-1	1.212-1	1.229-0	1.236-0	1.259-0	1.303-1	1.324-0	1.349-1	1.412-0	1.434-0	1.464-0	
4	1.104-1	1.159-1	1.212-0	1.234-0	1.264-0	1.283-1	1.322-0	1.377-0	1.359-0	1.392-0	1.446-0	
5	1.104-1	1.159-1	1.171-0	1.193-0	1.193-0	1.204-1	1.207-0	1.315-0	1.333-0	1.372-0	1.416-0	
VW	12	13	14	15	16	17	18	19	20	21	22	23
V	1.636-0	1.059-1	1.477-0	1.547-0	1.295-0	1.514-0	1.375-0	1.675-0	1.393-0	1.203-0	1.396-0	1.324-0
1	1.245-1	1.292-1	1.053-0	1.563-0	1.945-0	1.231-0	1.326-0	1.420-0	1.334-0	1.595-0	1.421-0	5.771-1
2	1.517-1	1.251-1	1.537-0	1.619-0	1.637-0	1.793-0	1.474-0	1.616-0	1.527-0	1.279-0	1.326-0	1.397-0
3	1.434-1	1.521-1	1.569-0	1.592-0	1.630-0	1.665-1	1.741-0	2.021-0	1.598-0	1.547-0	9.715-1	1.253-0
4	1.474-1	1.474-1	1.536-0	1.576-0	1.625-0	1.641-0	1.646-0	1.751-0	1.798-0	1.649-0	1.637-0	1.391-0
5	1.431-1	1.465-1	1.515-0	1.546-0	1.596-0	1.616-0	1.653-0	1.695-0	1.773-0	1.739-0	1.755-0	7.977-0

NOT REPRODUCIBLE

Table II5

2-CENTROIDS FOR (V) GAMMA PRIME I

V	VV	1	2	3	4	5	6	7	8	9	10	11
1	1.014-1	1.014-1	1.0357-0	1.0344-0	1.031-0	1.014-1	1.024-1	1.0224-1	1.0341-1	1.0247-1		
2	1.015-1	1.011-1	1.0136-0	1.0170-1	1.025-1	1.037-1	1.020-0	1.014-1	1.032-1	1.0463-1		
3	1.0152-1	1.015-1	1.0120-0	1.0139-1	1.031-0	1.035-1	1.014-0	1.027-1	1.031-0	1.034-1		
4	1.017-1	1.017-1	1.0144-0	1.0131-1	1.014-1	1.026-0	1.026-0	1.0274-0	1.017-1	1.0342-1		
5	1.024-1	1.024-1	1.0145-0	1.0151-1	1.015-0	1.0113-1	1.030-0	1.037-1	1.045-1	1.025-0	1.0303-0	
6	1.0235-1	1.0235-1	1.0211-0	1.0375-1	1.013-1	1.013-1	1.0129-0	1.028-1	1.0176-0	1.0153-0	1.0110-0	

V	VV	12	13	14	15	16	17	18	19	20	21	22	23
1	9.01-7-1	9.0135-1	3.0135-1	3.0398-1	9.0362-1	9.0451-1	9.0457-1	9.0451-1	7.0479-1	1.0302-0	1.0113-0	1.0172-0	
2	9.0336-1	9.0235-1	9.0153-1	9.0394-1	9.036-1	9.036-1	9.036-1	9.036-1	9.051-1	6.0587-1	1.0124-0	1.0923-0	
3	9.0544-1	9.0422-1	9.0393-1	9.0187-1	9.074-1	9.065-1	9.051-1	9.051-1	9.0756-1	8.0399-1	8.0366-1	7.0475-1	
4	9.07-1-1	9.0675-1	9.0477-1	9.0356-1	9.0240-1	9.0125-1	9.0125-1	9.0125-1	9.012-1	9.0579-1	9.0559-1	9.0365-1	
5	9.0942-1	9.0460-1	9.0672-1	9.0541-1	9.0416-1	9.0299-1	9.0199-1	9.0199-1	9.0921-1	8.0959-1	8.0947-1	8.0716-1	
6	9.1000-1	9.051-1	9.0405-1	9.0391-1	9.0612-1	9.0406-1	9.0353-1	9.0353-1	9.0255-1	9.0134-1	9.0134-1	8.0922-1	

Table III6
R-CENTROIDS FOR (NC FEAST 1)

<i>v</i>	<i>w</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>5</i>
0	1.096-3	1.0324-3	9.0313-1	9.05-7-1	1.0175-J	1.0039-J			
1	3.927-J	1.0375-0	9.0916-1	9.0321-1	4.0752-1	1.0114-J			
2	1.162-3	5.024-J	1.0033-0	3.0343-1	3.0279-1	9.0426-1			
3	9.140-1	1.0230-0	1.0131-J	1.0191-0	3.0156-0	8.0150-1			
4	1.196-3	1.0223-1	1.0359-0	1.0311-J	1.0150-0	2.0141-L			
5	1.035-3	1.0394-0	1.0123-J	1.0291-0	1.0310-0	1.0110-J			
6	9.532-1	3.0457-1	1.0343-J	2.0152-0	2.0179-0	1.0336-U			
7	9.570-1	9.0608-1	9.0224-1	1.0135-0	3.0152-0	0.0520-1			

Table III7
R-CENTROIDS FOR (NC FEAST 2)

<i>v</i>	<i>w</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>5</i>
0	1.069-0	1.0683-0	1.0374-0	3.0352-1	1.0124-0	1.0334-U			
1	4.916-1	1.076-	1.0367-J	1.0337-0	1.0193-J	1.0097-J			
2	1.231-0	5.297-1	1.0314-0	1.0372-0	1.0173-0	1.0246-U			
3	1.034-J	5.146-	3.0414-1	1.0332-0	1.0250-0	1.0127-J			
4	1.134-3	1.259-U	1.0419-1	3.0825-1	1.0100-0	1.0057-U			
5	1.034-J	1.0039-0	3.0233-0	1.0317-1	3.0166-1	1.0109-U			

Table III8

R-CENTROIDS FOR (NO L-H)

V	W	J	1	2	3	4	5	6	7
1	1.093-1	1.0531-1	1.0233-1	1.0123-1	1.0112-1	1.0154-1	2.0132-1	1.0077-1	
2	1.203-1	1.1723-1	1.0723-1	1.0094-1	1.0323-1	1.0123-1	1.0130-1	1.163-1	
3	1.125-1	1.020-1	1.0044-1	1.0033-1	1.0144-1	1.0343-1	1.0122-1	2.745-1	
4	1.331-1	7.012-1	2.0153-1	2.0193-1	2.0176-1	1.0212-1	2.0369-1	1.0667-1	
5	1.145-1	2.0032-1	3.0143-1	3.0221-1	1.0102-1	2.004-1	1.0574-1	4.0229-1	
6	1.0434-1	3.0234-1	3.0344-1	3.0569-1	1.0111-1	2.0712-1	9.0461-1		

NOT REPRODUCIBLE

Table III9

R-CENTROIDS FOR (NO L-H)

V	W	U	L	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
1	1.2+3-1	1.0291-1	1.0246-1	1.0344-1	1.0330-1	1.0323-1	1.0277-1	1.0411-1	1.0430-1	1.0452-1	1.0479-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	1.0509-1	
2	1.2412-1	1.0242-1	1.0273-1	1.0234-1	1.0315-1	1.0321-1	1.0355-1	1.0387-1	1.0421-1	1.0436-1	1.0461-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	1.0464-1	
3	1.0243-1	4.0234-1	1.0261-1	1.0239-1	1.0314-1	1.0327-1	1.0348-1	1.0389-1	1.0415-1	1.0422-1	1.0446-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	1.0472-1	
4	1.0249-1	1.0221-1	1.0248-1	1.0247-1	1.0312-1	1.0312-1	1.0312-1	1.0312-1	1.0341-1	1.0412-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1	1.0529-1		
5	1.0117-1	4.0214-1	1.0259-1	1.0234-1	1.0279-1	1.0279-1	1.0274-1	1.0324-1	1.0343-1	1.0357-1	1.0393-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	1.0412-1	
6	1.0137-1	1.0217-1	1.0247-1	1.0205-1	1.0205-1	1.0231-1	1.0314-1	1.0314-1	1.0314-1	1.0356-1	1.0375-1	1.0397-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	1.0424-1	
7	1.0117-1	1.0216-1	1.0235-1	1.0259-1	1.0274-1	1.0293-1	1.0293-1	1.0293-1	1.0324-1	1.0349-1	1.0364-1	1.0394-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	1.0404-1	
8	1.0113-1	1.0205-1	1.0222-1	1.0222-1	1.0266-1	1.0266-1	1.0266-1	1.0266-1	1.0291-1	1.0315-1	1.0354-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1	1.0371-1		

Table I20

R-CENTROIDS FOR (002) S-R

VV	J	1	2	3	4	5	6	7	8	9	10	11
y	1.374-3	1.0361-3	1.0434-3	1.0419-3	1.0435-3	1.0427-3	1.0430-3	1.0433-3	1.0436-3	1.0534-3	1.0553-3	
1	1.374-3	1.0362-3	1.0377-3	1.0412-3	1.0426-3	1.0458-3	1.0474-3	1.0491-3	1.0500-3	1.0525-3	1.0542-3	
2	1.352-3	1.0371-3	1.0392-3	1.0415-3	1.0426-3	1.0455-3	1.0492-3	1.0498-3	1.0515-3	1.0530-3	1.0539-3	
3	1.350-3	1.0371-3	1.0394-3	1.0413-3	1.0424-3	1.0443-3	1.0450-3	1.0474-3	1.0490-3	1.0503-3	1.0537-3	
4	1.351-3	1.0364-3	1.0378-3	1.0393-3	1.0407-3	1.0422-3	1.0437-3	1.0451-3	1.0466-3	1.0494-3	1.0514-3	
5	1.345-3	1.0357-3	1.0387-3	1.0411-3	1.0430-3	1.0445-3	1.0450-3	1.0464-3	1.0473-3	1.0486-3	1.0493-3	
6	1.335-3	1.0354-3	1.0367-3	1.0381-3	1.0395-3	1.0424-3	1.0439-3	1.0454-3	1.0465-3	1.0478-3	1.0485-3	
7	1.335-3	1.0343-3	1.0362-3	1.0370-3	1.0390-3	1.0416-3	1.0430-3	1.0454-3	1.0465-3	1.0478-3	1.0485-3	
8	1.332-3	1.0344-3	1.0352-3	1.0371-3	1.0395-3	1.0412-3	1.0435-3	1.0445-3	1.0458-3	1.0471-3	1.0489-3	
9	1.327-3	1.0341-3	1.0354-3	1.0367-3	1.0380-3	1.0394-3	1.0426-3	1.0439-3	1.0452-3	1.0455-3	1.0486-3	
10	1.323-3	1.0337-3	1.0350-3	1.0363-3	1.0376-3	1.0389-3	1.0398-3	1.0421-3	1.0433-3	1.0446-3	1.0471-3	
11	1.325-3	1.0335-3	1.0346-3	1.0359-3	1.0372-3	1.0385-3	1.0415-3	1.0426-3	1.0435-3	1.0462-3	1.0474-3	
12	1.317-3	1.0331-3	1.0343-3	1.0356-3	1.0369-3	1.0381-3	1.0414-3	1.0424-3	1.0433-3	1.0456-3	1.0469-3	
13	1.315-3	1.0321-3	1.0341-3	1.0353-3	1.0366-3	1.0377-3	1.0398-3	1.0418-3	1.0446-3	1.0452-3	1.0464-3	
14	1.312-3	1.0325-3	1.0339-3	1.0351-3	1.0364-3	1.0373-3	1.0394-3	1.0415-3	1.0439-3	1.0449-3	1.0460-3	
15	1.311-3	1.0324-3	1.0336-3	1.0349-3	1.0362-3	1.0367-3	1.0392-3	1.0413-3	1.0412-3	1.0435-3	1.0454-3	
16	1.319-3	1.0322-3	1.0335-3	1.0348-3	1.0360-3	1.0367-3	1.0394-3	1.0411-3	1.0432-3	1.0444-3	1.0443-3	
17	1.313-3	1.0321-3	1.0334-3	1.0347-3	1.0359-3	1.0362-3	1.0395-3	1.0400-3	1.0431-3	1.0442-3	1.0327-3	
18	1.317-3	1.0321-3	1.0333-3	1.0346-3	1.0356-3	1.0361-3	1.0397-3	1.0398-3	1.0429-3	1.0443-3	1.0457-3	
19	1.317-3	1.0319-3	1.0332-3	1.0345-3	1.0357-3	1.0366-3	1.0397-3	1.0400-3	1.0429-3	1.0439-3	1.0472-3	
20	1.316-3	1.0319-3	1.0332-3	1.0344-3	1.0356-3	1.0359-3	1.0395-3	1.0423-3	1.0429-3	1.0439-3	1.0467-3	

NOT REPRODUCIBLE

Table I20 (cont'd)

(C2) 5-21

V	VV	12	13	14	15	16	17	18	19	20	21	22	23
1	1.512-	1.0291-	1.0012-L	1.0034-	1.0057-0	1.0074-	1.0093-	1.0093-	1.0074-	1.0055-0	1.0033-0	1.0010-	1.0035-0
2	1.513-	1.0272-	1.0124-	1.0027-	1.0046-0	1.0027-	1.0051-0	1.0073-	1.0073-	1.0065-	1.0073-	1.0029-	1.0029-
3	1.413-	1.0272-	1.0592-L	1.0514-	1.0629-0	1.0514-	1.0535-0	1.0717-	1.0717-	1.0727-0	1.0514-	1.0404-	1.0404-
4	1.512-	1.0160-	1.0577-L	1.028-	1.0028-0	1.0044-	1.0044-	1.0655-	1.0655-	1.0602-0	1.0741-	1.0765-	1.0791-
5	1.513-	1.0164-	1.0534-	1.0534-	1.0616-0	1.0627-	1.0536-0	1.0675-	1.0675-	1.0639-0	1.0720-	1.0730-	1.0794-
6	1.512-	1.0152-	1.0577-	1.0565-	1.0533-	1.0533-	1.0533-	1.0611-	1.0611-	1.0632-0	1.0679-	1.0711-	1.0753-
7	1.513-	1.0152-	1.0533-	1.0523-	1.0523-	1.0523-	1.0523-	1.0594-	1.0594-	1.0528-0	1.0517-	1.0678-	1.0765-
8	1.512-	1.0152-	1.0521-	1.0540-L	1.0527-	1.0534-	1.0534-	1.0593-	1.0593-	1.0716-	1.0645-	1.0663-	1.0733-
9	1.513-	1.0151-	1.0521-	1.0531-	1.0553-	1.0553-	1.0553-	1.0572-	1.0572-	1.0617-	1.0631-	1.0679-	1.0706-
10	1.419-	1.0150+	1.0538-	1.0538-	1.0544-	1.0556-	1.0556-	1.0592-	1.0592-	1.0535-0	1.0611-	1.0653-0	1.0667-
11	1.512-	1.0123-	1.0528-	1.0539-	1.0532-	1.0532-	1.0532-	1.0590-	1.0590-	1.0592-0	1.0632-	1.0639-	1.0653-
12	1.513-	1.0121-	1.0521-	1.0521-	1.0521-	1.0521-	1.0521-	1.0571-	1.0571-	1.0571-	1.0614-	1.0629-	1.0634-
13	1.412-	1.0120-	1.0505-	1.0514-	1.0567-	1.0552-	1.0552-	1.0592-	1.0592-	1.0533-	1.0605-	1.0611-	1.0655-
14	1.512-	1.0149-	1.0494-	1.0517-	1.0534-	1.0546-	1.0546-	1.0546-	1.0546-	1.0546-	1.0546-	1.0575-	1.0642-
15	1.413-	1.0143-	1.0494-	1.0475-	1.0535-	1.0535-	1.0535-	1.0525-	1.0525-	1.0579-	1.0626-	1.0635-	1.0642-
16	1.412-	1.0143-	1.0494-	1.0494-	1.0528-	1.0532-	1.0532-	1.0571-	1.0571-	1.0632-	1.0639-	1.0653-	1.0667-
17	1.413-	1.0142-	1.0485-	1.0515-	1.0522-	1.0522-	1.0522-	1.0559-	1.0559-	1.0567-	1.0609-	1.0617-	1.0652-
18	1.412-	1.0142-	1.0485-	1.0485-	1.0514-	1.0516-	1.0516-	1.0555-	1.0555-	1.0555-	1.0609-	1.0615-	1.0649-
19	1.413-	1.0141-	1.0482-	1.0482-	1.0515-	1.0515-	1.0515-	1.0553-	1.0553-	1.0553-	1.0602-	1.0607-	1.0646-
20	1.412-	1.0141-	1.0482-	1.0482-	1.0515-	1.0515-	1.0515-	1.0552-	1.0552-	1.0552-	1.0601-	1.0606-	1.0653-

APPENDIX IV

ADDITIONAL TABLES FOR BIRGE-HOPFIELD TABLES

The purpose of this appendix is to supplement data appearing in the main text of this technical report. New data has been published and these data have been incorporated into the tables of Franck-Condon factors included in this report. To minimize the changes to the main body of the report, these data are being included in this appendix.

The confusing and contradictory tangle of excited states for the very high energies in the nitrogen molecule has been unraveled (Refs. 41, 42, 43). Dressler (Ref. 41) reports that the former twenty states of excited nitrogen can be regrouped into three valence states and three Rydberg states. The three valence states are the $b^1\pi_u$, $b'^1\Sigma_u^+$, and d' . It will be noted that the first two states are those associated with the Birge-Hopfield band systems which are pertinent to this report. The renumbering of the levels of these states has vastly increased the number of vibrational levels for the upper states of each of these systems. This necessitated recalculating the vibrational transition probabilities. The input data used to calculate the vibrational potential for the $b'^1\Sigma$ state was the deperturbed spectroscopic constants of Dressler. These data are listed in table 121. For the input data needed for the $b^1\pi$ state, the data given by Carroll and Collins was graphically smoothed and used. These smoothed data are listed in table 122. The potentials resulting from these data are listed in tables 123 and 124. The potentials were generated using program TURNGPT. The vibrational transition probabilities were calculated using program FRANKON. The Franck-Condon factors are listed in tables 60 and 61.

Table 121

SPECTROSCOPIC CONSTANTS FOR THE $N_2 b' ^1 \Sigma_u^+$ STATE

<u>v</u>	<u>G_v</u>	<u>B_v</u>
0	371.9	1.151
1	1112.0	1.143
2	1848.0	1.135
3	2580.0	1.127
4	3308.0	1.119
5	4031.0	1.111
6	4750.0	1.103
7	5464.0	1.095
8	6174.0	1.087
9	6879.0	1.079
10	7580.0	1.071
11	8276.0	1.063
12	8960.0	1.055
13	9632.0	1.047
14	10292.0	1.039
15	10940.0	1.031
16	11576.0	1.023
17	12200.0	1.015
18	12812.0	1.007
19	13412.0	0.999
20	14099.0	0.991

Table 122

POTENTIAL ENERGY FOR THE $N_2 b' ^1 \Sigma_u^+$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	371.9	1.3672	1.5282	0.0461
1	1112.0	1.3158	1.5953	0.1380
2	1848.0	1.2825	1.6443	0.2292
3	2580.0	1.2568	1.6859	0.3199
4	3308.0	1.2355	1.7231	0.4102
5	4031.0	1.2170	1.7576	0.4999
6	4750.0	1.2007	1.7899	0.5890
7	5464.0	1.1861	1.8207	0.6775
8	6174.0	1.1729	1.8501	0.7655
9	6879.0	1.1607	1.8786	0.8529
10	7580.0	1.1495	1.9061	0.9398
11	8276.0	1.1389	1.9333	1.0261
12	8960.0	1.1283	1.9612	1.1109
13	9632.0	1.1181	1.9889	1.1942
14	10292.0	1.1083	2.0167	1.2761
15	10940.0	1.0988	2.0445	1.3564
16	11576.0	1.0896	2.0723	1.4352
17	12200.0	1.0807	2.1001	1.5126
18	12812.0	1.0719	2.1283	1.5885
19	13412.0	1.0640	2.1552	1.6629
20	14099.0	1.0701	2.1504	1.7480

Table 123

POTENTIAL ENERGY FOR THE $N_2 b^1 \pi_u$ STATE

<u>v</u>	<u>V(cm⁻¹)</u>	<u>r_{min}</u>	<u>r_{max}</u>	<u>V(ev)</u>
0	313.2	1.2053	1.3819	0.0388
1	947.0	1.1553	1.4540	0.1174
2	1632.0	1.1288	1.5031	0.2024
3	2354.0	1.1090	1.5445	0.2918
4	3110.0	1.0969	1.5792	0.3856
5	3889.0	1.0859	1.6121	0.4822
6	4682.0	1.0765	1.6437	0.5805
7	5481.0	1.0687	1.6751	0.6794
8	6278.0	1.0616	1.7063	0.7784
9	7063.0	1.0550	1.7390	0.8757
10	7831.0	1.0490	1.7725	0.9708
11	8578.0	1.0432	1.8070	1.0635
12	9303.0	1.0382	1.8426	1.1533
13	10004.0	1.0337	1.8794	1.2403
14	10682.0	1.0298	1.9169	1.3243
15	11337.0	1.0263	1.9555	1.4055
16	11967.0	1.0231	1.9954	1.4836
17	12575.0	1.0206	2.0359	1.5590
18	13159.0	1.0182	2.0780	1.6314
19	13719.0	1.0162	2.1216	1.7009
20	14255.0	1.0150	2.1672	1.7673
21	14768.0	1.0147	2.2149	1.8309
22	15257.0	1.0135	2.2652	1.8915

Table 124

SPECTROSCOPIC CONSTANTS FOR THE $N_2 b^1 \pi_u$ STATE

<u>v</u>	<u>G_v</u>	<u>B_v</u>
0	313.2	1.442
1	947.0	1.424
2	1632.0	1.400
3	2354.0	1.376
4	3110.0	1.359
5	3889.0	1.334
6	4682.0	1.313
7	5481.0	1.286
8	6278.0	1.263
9	7063.0	1.235
10	7831.0	1.208
11	8578.0	1.181
12	9303.0	1.150
13	10004.0	1.120
14	10682.0	1.089
15	11337.0	1.059
16	11967.0	1.028
17	12575.0	0.997
18	13159.0	0.966
19	13719.0	0.934
20	14255.0	0.898
21	14768.0	0.860
22	15257.0	0.819

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13. ABSTRACT

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In the process of calculating opacities which are needed as input data for radiation transport problems, the absorption cross sections for various species has to be known. One factor in the cross section is the vibrational transition probability, called the Franck-Condon factor (FCF). This report presents input data needed to calculate these from Rydberg-Klein potentials as well as tables of Franck-Condon factors for species of atmospheric interest. ()

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Vibrational transition probabilities						
Franck-Condon factors						
Vibrational potential						
Rydberg-Klein potential						
N ₂						
O ₂						
NO						
CO						
CN						
N ₂ ⁺						
O ₂ ⁺						
Photoionization Franck-Condon factors						
Computer program						

UNCLASSIFIED

Security Classification